An Euler-Lagrange analysis of turbulent two-phase mixing in a vertical pipe in a Star-CD environment

by Mark Moonen

Technische Universität Berlin
Institut für Verfahrenstechnik
Supervisor: Prof. Dr.-Ing. M. Kraume
Dr. Anja Paschedag
Dr. Alberto Varone
Dipl.-Ing. Manfredi Signorino
Technische Universiteit Delft
Kramers Laboratorium voor Fysische Technologie
Supervisor: Prof. Dr. H. van den Akker
Dr. Jos Derksen
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Summary

Within the framework of the European Union PRATSOLIS project, an analysis of turbulent two-phase mixing in a vertical pipe by the commercial CFD code Star-CD environment has been performed. The aim of this study was to assess whether and how simulations of pipe flow can be performed in Star-CD, to create a Star-CD mesh of the pipe-flow for one- and two-phase flow simulation and to analyze Signorino’s experimental results. On the basis of experimental results taken from literature, Star-CD has been validated. It performs well for one-phase flow, but not for dilute two-phase flow. The reason for this is that Star-CD does not take turbulence modulation into account, nor can Star-CD be modified to do so. Signorino’s one-phase experimental data have been qualitatively well simulated. The obstruction of the flow due to the measuring device and the absence of accurate inlet conditions, makes a quantitatively correct simulation infeasible.
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Chapter 1

Introduction

1.1 PRATSOLIS

This thesis is a report of the work done between March 2002 and January 2003 at the TU Berlin and TU Delft, within the frame of the PRATSOLIS project. The acronym PRATSOLIS stands for PRecipitation and Agglomeration in Turbulent SOLid Liquid Systems and is a project with the aim to contribute to the development and implementation of models that can be integrated in computational fluid dynamics (CFD) codes and permit the prediction of precipitation and agglomeration in the typical complex systems which are met in industrial plants. The case of high solid volume fraction is particularly investigated.

Precipitation, also cited as reactive crystallization, consists in the mass crystallization of small solid particles by a phase transition from super-saturated solution to the solid phase. Agglomeration is the process of formation of one particle out of smaller particles.

The relevant point of the investigation of the PRATSOLIS-project to this study is the fluid-particle interaction. This point includes the analysis of what is usually called one-way, two-way and four-way interaction between particles and turbulence. One-way interaction points to the prevailing action of dispersion of particles exerted by the turbulent fluid on the particles. If the solid volume fraction is sufficiently high, the wakes generated by the particles modify the structure of turbulence and, in turn, affect the dispersion giving rise to two-way coupling. At even higher volume fractions, particle-particle collisions, particle-wall collisions and overlap of the wakes become important and modify further the turbulence structure, originating in four-way coupling. It should be noted that, although the interaction between fluid and particles is of hydrodynamic nature, it affects are those phenomena that are modulated by turbulence as, for instance, the rate of fast reactions, nucleation and growth of crystals, coagulation and breakage kinetics, and the resulting morphology of particles. More information about PRATSOLIS can be found at the web-site: http://www.esme.fr/pratsolis.
1.2 TU-Berlin Group

The group working on the PRATSOLIS project at the TU-Berlin consists of Manfredi Signorino, Alberto Varone, Anja Paschendag and Matthias Kraume. The experimental work of Signorino is focussed on the fluid-particle interaction for dense steady-state flows. He studies the effect of the addition of particles on the mixing of two in temperature differing water streams in a vertical downward pipe flow. Measurements of the radial temperature profiles at different axial positions at different volume fractions of particles are done intrusively using thermocouples, which are fixed at a radial position on a cross.

Simulations of one-phase and two-phase flow are performed, using the commercial CFD-code Star-CD. Star-CD developed a framework for dispersed multi-phase flow, such as can be found in liquid- and solid-fuelled combustors, spray driers, cyclone dust separators and chemical reactors. Mostly large scale equipment, in which the calculation of the particle trajectories is of main importance. In all cases the flow consists of a continuous phase and one or more dispersed phases in the form of particles. The motion of the dispersed phase will be effected by that of the continuous one and vice versa via displacement and inter-phase momentum, mass and heat transfer effects. The strength of the interactions will depend on the dispersed phase particle's size, density and number density. Next to this Star-CD provides models for particle-particle collisions and particle-wall collisions.

The emphasis of the current work of the TU-Berlin group does not lay on the correct calculation of the particle trajectories, but on the effect of the particles on turbulence. Therefore Star-CD will have to be tested and possibly adapted to calculate this effect correctly.

1.3 The aim of this study

The aim of this study is to support Signorino's experimental work by simulation in the Star-CD environment: to assess whether and how two-phase simulations of the pipe flow can be performed in Star-CD, to create a Star-CD mesh of the pipe-flow for one- and two-phase flow simulation and to analyze Signorino's experimental results.

1.4 Setup of the thesis

Two-phase turbulent flow description relies heavily on one-phase turbulent flow description. Therefore one-phase turbulent flow is treated in chapter 2, followed by turbulent two-phase flow in chapter 3. To perform simulations with the model equations derived in chapter 2 and 3, they are converted into algebraic relations, which are solved in numerical algorithms. This is presented in chapter 4. In chapter 5 the implementation of multiphase turbulent flow in Star-CD is treated, with an emphasis on the differences with the model equations, algebraic relations and numerical algorithms presented in the previous three chapters. In chapter 6 the results are presented of the assessment of Star-CD two-phase simulation capabilities, of the
1.4. SETUP OF THE THESIS

mesh construction for two-phase flow and of the preliminary analysis of Signorino's experimental results. The conclusions are presented in chapter 7.
Chapter 2

One-Phase Flow

In the first section (2.1) some words will be spent on the phenomenon of turbulence and the basic quantification of turbulence in scales and dimensional quantities. Turbulent one-phase flow of an incompressible fluid can be described using a set of four equations: the continuity equation and the three Navier-Stokes equations. For the description of the temperature field the thermal energy equation is used. They will be derived in section 2.2.

However, the flow field can not be resolved down to the smallest scale of turbulence for highly turbulent flows. Therefore the equations will have to be transformed into their averaged counterparts (section 2.3). This gives rise to averaged products of fluctuations. These new terms are the Reynolds stresses and the turbulent scalar fluxes.

These can be modelled using the Boussinesq assumption and analogs (section 2.4). The turbulent viscosity, which is introduced in the Boussinesq assumption can be calculated from the turbulent kinetic energy $k$ and the turbulent energy dissipation $\epsilon$. An equation to describe the turbulent kinetic energy, including the definition of $\epsilon$, is derived in section 2.5. In section 2.6 the standard k-\(\epsilon\) model and Chen’s k-\(\epsilon\) model are presented.

The averaged continuity, averaged Navier-Stokes, averaged thermal energy and the k-\(\epsilon\) model form a closed set of equations that can be solved numerically, which describe one-phase, thermally varying, non-reactive flow. They are summarized and put into general form in section 2.7.

2.1 Turbulence Description

A basic distinction in fluid dynamics is the distinction between laminar and turbulent flow. In laminar flow the flow can be thought of as a collection of laminae, where each lamina slides with constant velocity between two other laminae. In a confined flow such as pipe flow a laminar flow can be realized, when the throughput is low enough. At the wall the cylindrical fluid lamina has no velocity, while the center lamina has the maximum velocity. Due to friction between the laminae, the resulting velocity profile in the radial direction is parabolic.

When the throughput $\phi_v$ is increased, there will be a point at which the friction...
can no longer level the velocity gradient and turbulence kicks in. The flow stumbles over slower parts of the fluid, creating non-laminar motion. The Reynolds number is defined as:

\[ Re = \frac{\rho Ud}{\mu} \]  

(2.1)

where \( D \) is the pipe diameter, \( \rho \) is the fluid density, \( \mu \) is the fluid viscosity and \( U = \phi_0/(\pi D^2) \) is the superficial velocity. The magnitude of this dimensionless group gives an indication of the relative importance of inertial and viscous fluid forces. When the viscous fluid force dominates the flow is laminar, when the inertial force is dominant the flow is turbulent. Pipe flow is fully turbulent for \( Re > 2.1 \cdot 10^3 \) [1].

When laminar pipe flow can be characterized by fluid cylinders sliding at constant speed in and over other cylinders, turbulent flow is characterized by eddy structures. An eddy is a swirling motion through the flow. Due to their motion they produce eddies of a smaller scale, which in turn produce smaller scaled eddies, down to a scale at which the velocity gradient is small enough to be handled by molecular viscosity.

Thus in the turbulent regime kinetic energy is transferred to turbulent kinetic energy \( k \) in the form of circulatory motion. The turbulent kinetic energy \( k \) flows down a cascade of ever in size decreasing eddies, until an eddy size at which the molecular dissipation can catch up again. In steady-state the rate of kinetic energy \( k \) flowing down this cascade is equal to the turbulent energy dissipation \( \epsilon \).

Dimensional analysis led Kolmogorov [2] to the definition of the time scale \( t_K \), the length scale \( l_K \) and the velocity scale \( u_K \) of the smallest eddies:

\[ t_K = \left( \frac{\nu}{\epsilon} \right)^{1/2} \]  

(2.2)

\[ l_K = \left( \frac{\nu^3}{\epsilon} \right)^{1/4} \]  

(2.3)

\[ u_K = \left( \frac{\nu \epsilon}{k} \right)^{1/4} \]  

(2.4)

Where \( \nu = \mu/\rho \) is the kinematic viscosity, \( \mu \) is the molecular viscosity and \( \rho \) is the fluid density. Defining a smallest eddy Reynolds number as

\[ Re_K = \frac{u_K l_K}{\nu} = 1, \]

shows the flow of the smallest eddy to be truly laminar, being viscously dissipated in a time \( t_K \).

Contrary to laminar flow, the velocity at one point is not constant. Depending on the passage of an eddy, the velocity at a point is a random variable. Because of this chaotic nature of turbulence it is not possible to predict the instantaneous velocity of a particular flow. Turbulence description is therefore stochastic and deals with averages and variations around averages.
2.1.1 Turbulence Description with numerical simulations

In computational fluid dynamics (CFD) the flow field is taken as space and time dependent changing of variables governed by conservation equations. These equations will be derived in the following sections. Space and time are discretized into finite elements, giving rise to a grid. By solving the governing equations together with the boundary conditions, particular to a certain flow, the flow field can be calculated. This type of computation is called Direct Numerical Simulation (DNS) and is computationally quite intensive. At the present it is only possible for relatively low Reynolds numbers, because DNS has to resolve down to the scales of the smallest eddies. These scales decrease with increasing turbulence, demanding more computing power, thereby limiting the application of DNS.

To describe stronger turbulent flows, time and space are discretized into elements larger than the Kolmogorov scales. This means that the Navier-Stokes equations, which will be derived in section 2.2, cannot be used, because they refer to a point in the flow. When the flow is resolved beyond the smallest structure, they can be resolved numerically, but another set of equations is needed for coarser grids. This set is generated by averaging the Navier-Stokes equations. However the averaged variables are influenced by the effect of the fluctuations from average. This effect has to be accounted for. An example of fluctuations, which have an effect on the averaged variables, are the Reynolds stresses. The Reynolds stresses account for the turbulent momentum transport, due to the velocity fluctuations. The modelling of the Reynolds stresses by averaged strains on the finite grid elements is treated in section 2.4. With the modelling of the averaged products of fluctuations two other scalars are introduced: the turbulent kinetic energy $k$ and its dissipation $\varepsilon$. Next to the continuity, the three velocity component and the thermal energy transport equations, two other transport equations will be needed for the new scalars. Sections 2.5 and 2.6 treat the derivation of these equations of change.

When the turbulent flow field has (locally) in every direction the same turbulent characteristics, it is called (locally) isotropic. Isotropic turbulence is invariant to the interchanging of the space-directions, allowing a simplification of the description. When the turbulent flow field has the same characteristics over a spatial distance, it is called homogeneous turbulence. This allows the use of finite volumes for the description of the space dependence of the flow field.

2.2 Mass, Momentum and Thermal Energy Balances over a Box

In this section the continuity, the Navier-Stokes equations and the change of thermal energy will be derived by writing the mass, momentum and thermal energy balances over a box.

Over a box of finite dimensions $\Delta x \ \Delta y \ \Delta z$ at $x$, $y$, $z$ the mass balance is:

$$\text{change of mass} = \text{mass flow}_{\text{in}} - \text{mass flow}_{\text{out}}$$
\[ \Delta (\rho \Delta x \Delta y \Delta z) \Delta t = \left( u_x \rho \Delta y \Delta z \right)_{x+\Delta x} - \left( u_x \rho \Delta y \Delta z \right)_{x} + \left( u_y \rho \Delta x \Delta z \right)_{y+\Delta y} - \left( u_y \rho \Delta x \Delta z \right)_{y} + \left( u_z \rho \Delta x \Delta y \right)_{z+\Delta z} - \left( u_z \rho \Delta x \Delta y \right)_{z} \] (2.5)

Where \( \rho \) is the fluid density and \( u_x, u_y, u_z \) are the velocity components in respectively the \( x, y \) and \( z \) direction.

Shrinking the dimensions of the box and the time of change to almost zero, using \( \frac{\partial f}{\partial x} = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x} \) and rearranging, this becomes:

\[ \frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_x)}{\partial x} + \frac{\partial (\rho u_y)}{\partial y} + \frac{\partial (\rho u_z)}{\partial z} = 0 \] (2.6)

Using the Einstein convention:

\[ \frac{\partial u_i}{\partial x_i} = \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} \] (2.7)

where \( i, j = 1, 2, 3 \) and \( x_1 = x, x_2 = y, x_3 = z \), gives the continuity-equation:

\[ \frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0 \] (2.8)

If the flow is incompressible, as can be assumed for a liquid, \( \rho = \text{constant} \). This reduces the continuity equation for incompressible flow to:

\[ \frac{\partial u_i}{\partial x_i} = 0 \] (2.9)

The incompressible continuity equation couples gradients of the different velocity-components and is used in the derivation of the Navier-Stokes equation.

Over a box of finite dimensions \( \Delta x \Delta y \Delta z \) at \( x, y, z \) the \( x \)-momentum-balance is:

\[ \text{change of momentum}_x = \text{momentum}_x \text{flow}_{\text{in}} - \text{momentum}_x \text{flow}_{\text{out}} + \text{forces}_x \]

The forces considered are pressure, gravity and friction.

\[ \Delta (\rho u_x \Delta x \Delta y \Delta z) \Delta t = u_x u_x \rho \Delta y \Delta z \bigg|_{x+\Delta x} - u_x u_x \rho \Delta y \Delta z \bigg|_{x} + u_y u_y \rho \Delta x \Delta z \bigg|_{y+\Delta y} - u_y u_y \rho \Delta x \Delta z \bigg|_{y} + u_z u_z \rho \Delta x \Delta y \bigg|_{z+\Delta z} - u_z u_z \rho \Delta x \Delta y \bigg|_{z} \]
2.2. MASS, MOMENTUM AND THERMAL ENERGY BALANCES OVER A BOX

\[ + u_x u_z \rho \Delta x \Delta y \bigg|_{z} - u_x u_z \rho \Delta x \Delta y \bigg|_{z+\Delta z} + \\
+ \tau_{xz} \Delta y \Delta z \bigg|_{x} - \tau_{xz} \Delta y \Delta z \bigg|_{x+\Delta x} + \\
+ \tau_{yz} \Delta x \Delta z \bigg|_{y} - \tau_{yz} \Delta x \Delta z \bigg|_{y+\Delta y} + \\
+ \tau_{zx} \Delta x \Delta y \bigg|_{z} - \tau_{zx} \Delta x \Delta y \bigg|_{z+\Delta z} + \\
+ p_x \Delta y \Delta z \bigg|_{z} - p_x \Delta y \Delta z \bigg|_{z+\Delta z} + \\
\rho g_x \Delta x \Delta y \Delta z \] (2.10)

With the dimensions of the box and the change of time approaching zero and rearranging, gives:

\[
\frac{\partial (\rho u_x)}{\partial t} = \frac{\partial (\rho u_x u_z)}{\partial x} - \frac{\partial (\rho u_y u_z)}{\partial y} - \frac{\partial (\rho u_z u_x)}{\partial z} + \\
- \frac{\partial \tau_{xz}}{\partial x} - \frac{\partial \tau_{yz}}{\partial y} - \frac{\partial \tau_{zx}}{\partial z} + \\
- \frac{\partial p}{\partial x} + \rho g_x 
\] (2.11)

Using suffix notation this can be generalized to the Navier-Stokes equation for compressible flow:

\[
\frac{\partial (\rho u_i)}{\partial t} = - \frac{\partial (\rho u_j u_i)}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial p}{\partial x_i} + \rho g_i 
\] (2.12)

Assuming the fluid is Newtonian, the stress tensor is linearly dependent on the velocity gradient. Using Newton’s law of viscosity [1]: \( \tau_{ij} = -\mu \frac{\partial u_i}{\partial x_j} \), assuming \( \rho = \text{constant} \) and rearranging using the continuity equation 2.9, gives the Navier-Stokes equation for single-phase constant density flows:

\[
\frac{\partial u_i}{\partial t} = -u_j \frac{\partial u_i}{\partial x_j} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} - \frac{1}{\rho} \frac{\partial p}{\partial x_i} + g_i 
\] (2.13)

The first term on the right-hand side of the equation represents the change of the velocity-component due to convective momentum transport, the second due to molecular transport of momentum and the third and fourth due to the pressure-gradient and gravity.

Over a box of finite dimensions \( \Delta x \Delta y \Delta z \) at \( x, y, z \) the thermal energy balance for incompressible flow is:

\[
\text{change of thermal energy} = \text{thermal energy flow in} + \\
- \text{thermal energy flow out} + \\
+ \text{thermal energy produced by friction}
\]
The energy flux is divided into convection and conduction. The convective flux is due to the fluid motion, the conductive flux \( q_i \) is due to a thermal energy gradient. The kinetic energy loss due to the levelling of velocity differences by friction is equal to the thermal energy production.

\[
\Delta(c_p T \rho \Delta x \Delta y \Delta z) = c_p T u_x \rho \Delta y \Delta z \left|_{x}^{x+\Delta x} \right. - c_p T u_x \rho \Delta y \Delta z \left|_{x+\Delta x}^{x} \right. + \\
+ c_p T u_y \rho \Delta x \Delta z \left|_{y}^{y+\Delta y} \right. - c_p T u_y \rho \Delta x \Delta z \left|_{y+\Delta y}^{y} \right. + \\
+ c_p T u_z \rho \Delta x \Delta y \left|_{z}^{z+\Delta z} \right. - c_p T u_z \rho \Delta x \Delta y \left|_{z+\Delta z}^{z} \right. + \\
+ q_x \Delta y \Delta z \left|_{x}^{x+\Delta x} \right. - q_x \Delta y \Delta z \left|_{x+\Delta x}^{x} \right. + q_y \Delta x \Delta z \left|_{y}^{y+\Delta y} \right. + q_y \Delta x \Delta z \left|_{y+\Delta y}^{y} \right. + \\
- q_y \Delta x \Delta z \left|_{y}^{y+\Delta y} \right. + q_z \Delta x \Delta y \left|_{z}^{z+\Delta z} \right. - q_z \Delta x \Delta y \left|_{z+\Delta z}^{z} \right. + \\
- (u_x \tau_{xx} + u_y \tau_{yx} + u_z \tau_{xz}) \Delta y \Delta z \left|_{x}^{x+\Delta x} \right. + \\
+ (u_x \tau_{xx} + u_y \tau_{yx} + u_z \tau_{xz}) \Delta y \Delta z \left|_{x+\Delta x}^{x} \right. + \\
- (u_x \tau_{xy} + u_y \tau_{yy} + u_z \tau_{zy}) \Delta x \Delta z \left|_{y}^{y+\Delta y} \right. + \\
+ (u_x \tau_{xy} + u_y \tau_{yy} + u_z \tau_{zy}) \Delta x \Delta z \left|_{y+\Delta y}^{y} \right. + \\
- (u_x \tau_{xz} + u_y \tau_{yz} + u_z \tau_{zz}) \Delta x \Delta y \left|_{z}^{z+\Delta z} \right. + \\
+ (u_x \tau_{xz} + u_y \tau_{yz} + u_z \tau_{zz}) \Delta x \Delta y \left|_{z+\Delta z}^{z} \right. + \tag{2.14}
\]

With the dimensions of the box and the change of time approaching zero, constant density \( \rho \) and rearranging, gives:

\[
\frac{\partial(c_p T)}{\partial t} = -u_x \frac{\partial(c_p T)}{\partial x} - u_y \frac{\partial(c_p T)}{\partial y} - u_z \frac{\partial(c_p T)}{\partial z} + \\
- \frac{1}{\rho} \frac{\partial q_x}{\partial x} - \frac{1}{\rho} \frac{\partial q_y}{\partial y} - \frac{1}{\rho} \frac{\partial q_z}{\partial z} + \\
+ \frac{1}{\rho} \frac{\partial(u_x \tau_{xx} + u_y \tau_{yx} + u_z \tau_{xz})}{\partial x} + \\
+ \frac{1}{\rho} \frac{\partial(u_x \tau_{xy} + u_y \tau_{yy} + u_z \tau_{zy})}{\partial y} + \\
+ \frac{1}{\rho} \frac{\partial(u_x \tau_{xz} + u_y \tau_{yz} + u_z \tau_{zz})}{\partial z} + \tag{2.15}
\]

Using Fourier’s Law of Heat Conduction [1]: \( q_i = -\lambda \frac{\partial(c_p T)}{\partial x_i} \) and rearranging, gives
2.3 VARIABLE AVERAGING OVER TIME OR VOLUME

the equation of change of thermal energy:
\[ \frac{\partial (c_p T)}{\partial t} = -u_i \frac{\partial (c_p T)}{\partial x_i} + \lambda \frac{\partial^2 (c_p T)}{\partial x_i \partial x_j} + \frac{1}{\rho} \frac{\partial (u_i n_{ij})}{\partial x_j} \]  \hspace{1cm} (2.16)

Rewriting this equation using Newton’s Law of viscosity: \( \tau_{xixj} = -\mu \frac{\partial u_i}{\partial x_j} \), reveals the thermal energy source term as the result from the change of kinetic energy due to friction:
\[ \frac{\partial (c_p T)}{\partial t} = -u_i \frac{\partial (c_p T)}{\partial x_i} + \lambda \frac{\partial^2 (c_p T)}{\partial x_i \partial x_j} - \nu \frac{\partial^2 (u_i u_j)}{\partial x_j \partial x_j} \]  \hspace{1cm} (2.17)

2.3 Variable Averaging over Time or Volume

As mentioned in section 2.1 CFD makes use of grid-averaged variables, which equations contain the effect of fluctuations on the grid-averaged variables. The continuity, Navier-Stokes and thermal energy equations are derived for control volumes approaching zero volume, i.e. points in the flow field. So the point equations will be averaged over a finite time or over a finite volume, resulting in averaged flow-field properties such as the averaged velocity-components \( \overline{u_i} \) and the averaged thermal energy \( \overline{c_p T} \).

The local velocity can be decomposed in the average velocity and a velocity fluctuation due to the presence of eddies. For time this is known as Reynolds decomposition, more generally put:
\[ X = \overline{X} + X', \quad \overline{X} = \overline{X} + \overline{X'} = \overline{X} + \overline{X'} \quad \text{thus} \quad \overline{X'} = 0 \]  \hspace{1cm} (2.18)

More general is the following formulation:
\[ \langle X \rangle = \frac{1}{Y} \int_0^Y XdY = \frac{1}{Y} \int_0^Y (\langle X \rangle + X')dY = \langle X \rangle + \frac{1}{Y} \int_0^Y X'dY \quad \text{thus} \quad \langle X' \rangle = 0 \]  \hspace{1cm} (2.19)

Where \( Y \) is a finite time or volume. In this thesis Reynolds notation will be used, with the remark that in all equations it can be interchanged with the more general notation.

For turbulent flow it is necessary to average the continuity equation 2.9, the Navier-Stokes equation 2.13 and the thermal equation 2.17. The averaged continuity equation becomes:
\[ \frac{\partial (\overline{u_i} + u'_i)}{\partial x_i} = \frac{\partial \overline{u_i}}{\partial x_i} = 0 \]  \hspace{1cm} (2.20)

Averaging of the Navier-Stokes equation (2.13):
\[ \frac{\partial (\overline{u_i} + u'_i)}{\partial t} = -\left( \overline{u_j} + u'_j \right) \frac{\partial (\overline{u_i} + u'_i)}{\partial x_j} + \nu \frac{\partial^2 (\overline{u_i} + u'_i)}{\partial x_j \partial x_j} + \frac{1}{\rho} \frac{\partial (\overline{p} + p')}{\partial x_i} + \overline{g_i} \]  \hspace{1cm} (2.21)
The averaging of the transport terms gives rise to the Reynolds-stresses:

\[
(\bar{u}_j + u'_j) \frac{\partial(\bar{u}_i + u'_i)}{\partial x_j} = \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} + u'_j \frac{\partial u'_i}{\partial x_j} =
\]

\[
= \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial(u'_j u'_i)}{\partial x_j} - u'_i \frac{\partial u'_j}{\partial x_j}
\]

\[
eq \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial u'_j u'_i}{\partial x_j}
\]

\[
\text{eq.2.9=0}
\]

Resulting in the Reynolds-averaged Navier-Stokes (RANS) equation:

\[
\frac{\partial \bar{u}_i}{\partial t} = -\bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} - \frac{1}{\rho} \frac{\partial p}{\partial x_i} + g_i - \frac{\partial u'_j u'_i}{\partial x_j}
\]

(2.23)

Averaging the thermal energy equation (2.17):

\[
\frac{\partial (c_p(T + T'))}{\partial t} = - \frac{(\bar{u}_i + u'_i)}{\partial x_i} \frac{\partial (c_p(T + T'))}{\partial x_i} + \frac{\lambda \frac{\partial^2 (c_p(T + T'))}{\partial x_i \partial x_i}}{\rho}
\]

\[
- \nu \frac{\partial^2}{\partial x_i \partial x_i} \left( \frac{1}{2}(\bar{u}_i + u'_i)^2 \right)
\]

(2.24)

The averaging of transport terms is analogue to 2.22, gives rise to the turbulent thermal energy fluxes:

\[
(\bar{u}_i + u'_i) \frac{\partial (c_p(T + T'))}{\partial x_i} = \bar{u}_i \frac{\partial c_pT}{\partial x_i} + \frac{\partial c_pT u'_i}{\partial x_i}
\]

(2.25)

And even more terms arise by averaging the thermal energy production term:

\[
\nu \frac{\partial^2}{\partial x_j \partial x_j} \frac{1}{2}(\bar{u}_i + u'_i)^2 = \nu \frac{\partial^2}{\partial x_j \partial x_j} \left( \frac{1}{2} \bar{u}_i^2 + u'_i^2 \right)
\]

(2.26)

Resulting in the averaged thermal energy equation:

\[
\frac{\partial c_pT}{\partial t} = - \bar{u}_i \frac{\partial c_pT}{\partial x_i} + \lambda \frac{\partial^2 c_pT}{\partial x_i \partial x_i} - \nu \frac{\partial^2}{\partial x_j \partial x_j} \left( \frac{1}{2} \bar{u}_i \bar{u}_i \right) +
\]

\[
- \frac{\partial c_pT u'_i}{\partial x_i} - \nu \frac{\partial^2}{\partial x_j \partial x_j} \left( \frac{1}{2} u'_i u'_i \right)
\]

(2.27)
2.4 The Boussinesq Assumption

After averaging the Navier-Stokes and the thermal energy equation some terms remain unclosed. The Reynolds stresses $\bar{u}_i\bar{u}_j$ and the turbulent thermal energy fluxes $c_p T' u'_i$ need modelling as mentioned before, thereby closing the system of equations. The Boussinesq assumption for $p$ constant is:

$$\bar{u}'_i\bar{u}'_j = -2\nu_t \bar{s}_{ij} + \frac{2}{3} k \delta_{ij} \quad (2.28)$$

Where $\delta_{ij}$ is the Kronecker delta:

$$\delta_{ij} = \begin{cases} 1 & \text{if } i=j \\ 0 & \text{if } i \neq j \end{cases} \quad (2.29)$$

$\bar{s}_{ij}$ represents the average strain terms:

$$\bar{s}_{ij} = \frac{1}{2} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \quad (2.30)$$

and $\nu_t$ the turbulent kinematic viscosity:

$$\nu_t \equiv C_\mu \frac{k^2}{\epsilon} \quad \text{where } C_\mu = 0.09 \quad [3] \quad (2.31)$$

Where $k$ and $\epsilon$ are respectively the turbulent kinetic energy and its dissipation rate. They will be treated in the sections 2.5 and 2.6. The turbulent viscosity $\mu_t = \rho \nu_t$ introduced with the Boussinesq assumption, gives in analogy to the molecular viscosity $\mu$ the turbulent fluxes as the product of a 'constant' and a gradient. In analogy to the Boussinesq assumption the turbulent thermal energy fluxes are:

$$c_p T' u'_i = -\frac{\nu_t}{Pr_t} \frac{\partial c_p T}{\partial x_i} \quad (2.32)$$

Where $Pr_t$ is the turbulent Prandtl number.

The modelling of the Reynolds stresses and turbulent scalar fluxes moves the closure problem to $k$ and $\epsilon$. In the next section the $k$ equation will be presented.

2.5 Turbulent Kinetic Energy, the $k$-equation.

The turbulent kinetic energy, i.e. energy contained in eddy motion, has a mass concentration of $k$:

$$k \equiv \frac{1}{2} \left( u'_x u'_x + u'_y u'_y + u'_z u'_z \right) = \frac{1}{2} u'_i u'_i \quad (2.33)$$

The change in $k$ can be rewritten as:

$$\frac{\partial k}{\partial t} = \frac{\partial \left( \frac{1}{2} u'_i u'_i \right)}{\partial t} = u'_i \frac{\partial u'_i}{\partial t} = u'_i \left( \frac{\partial u_i}{\partial t} - \frac{\partial \bar{u}_i}{\partial t} \right) \quad (2.34)$$
So to derive the $k$ equation, the manipulations of the Navier-Stokes equation (2.13) that are needed, are subsequently averaging of the Navier-Stokes equation, (resulting in 2.23,) deduction of the averaged equation from the Navier-Stokes equation, multiplication of the difference with the velocity fluctuation and finally averaging of the product. The derivation of the $k$-equation is presented in appendix A. The $k$-equation, which is identical to equation 5.132 of Pope [4], is:

$$\frac{\partial k}{\partial t} = -\overline{u_j \frac{\partial k}{\partial x_j}} + \frac{\partial}{\partial x_j} T_j + P - \epsilon$$ (2.35)

where

$$T_j = \frac{1}{2} u'_i u'_j + \overline{u'_i u'_j} - 2\nu \overline{s'_{ij}}$$ (2.36)

$$P = -\overline{u'_i u'_j} \frac{\partial u_i}{\partial x_j}$$ (2.37)

$$\epsilon = 2\nu \overline{s'_{ij} s'_{ij}}$$ (2.38)

$$s'_{ij} = \frac{1}{2} \left( \frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i} \right)$$ (2.39)

The first term on the right-hand side of 2.35 represents the scalar transport due to convection, the second term is transport due to turbulent scalar fluxes, $P$ is the turbulent energy production, $\epsilon$ is the turbulent energy dissipation and $s'_{ij}$ used in the definition of $\epsilon$ represent the fluctuations of the strain at a point.

### 2.6 The $k/\epsilon$-equations

Moving the closure problem introduced with the Reynolds stresses and the turbulent scalar fluxes to the turbulent viscosity, which is evaluated with $k$ and $\epsilon$, shifts the problem to two other terms involving averaged products of fluctuations: $\epsilon$ and $T_j$. These terms can be evaluated by solving a transport equation for them, or by modelling. Launder and Spalding [3] represent all third order correlation which appear in the $k$ equation (2.35) ‘in absence of superior knowledge’ by way of gradients of $k$. Thus

$$\frac{\partial T_j}{\partial x_j} = \frac{\partial}{\partial x_j} \left( D_k \frac{\partial k}{\partial x_j} \right)$$

where $D_k$ is an effective diffusion coefficient for the turbulence energy $k$, depending on the turbulence regime. They solve a transport equation for $\epsilon$. At high Reynolds numbers the transport equations for $k$ and $\epsilon$ may be expressed:

$$\frac{\partial k}{\partial t} = -\overline{u_j \frac{\partial k}{\partial x_j}} + \frac{\partial}{\partial x_j} \left( \nu_k \frac{\partial k}{\partial x_j} \right) + 2\nu s'_{ij} \frac{\partial u_i}{\partial x_j} - \epsilon$$ (2.40)

$$\frac{\partial \epsilon}{\partial t} = -\overline{u_j \frac{\partial \epsilon}{\partial x_j}} + \frac{\partial}{\partial x_j} \left( \nu_k \frac{\partial \epsilon}{\partial x_j} \right) +$$

$$+ C_{1\epsilon} \frac{\epsilon}{k} (2\nu s'_{ij} \frac{\partial u_i}{\partial x_j} - C_{2\epsilon} \frac{\epsilon^2}{k})$$ (2.41)
2.7. Final Form of the Model Equations for One-Phase Flow

Originally assessed by Launder and Spalding [3] for free turbulent flow the k-\( \varepsilon \) model could not represent some turbulent flow problems. The spreading rate of a round jet is over-predicted by more than 30\% and for the turbulent flow over a backwards facing step the re-attachment length is under-predicted by more than 25\%. Because the dissipation rate equation is highly empirical in nature, improvement of the model performance is usually achieved by modifying the dissipation rate equation. Chen [5] introduced an additional term in the \( \varepsilon \)-equation to add a second time scale of the production range of the turbulent kinetic energy spectrum. Hereby enabling the energy transfer mechanism of the turbulence model to respond to the mean strain more effectively.

\[
\frac{\partial \varepsilon}{\partial t} = -\bar{u}_j \frac{\partial \varepsilon}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \nu \frac{\partial \varepsilon}{\partial x_j} \right) + C_{c1} \frac{\varepsilon}{k} \left( 2\nu \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} \right) + C_{c2} \frac{\varepsilon}{k} + C_{c3} \nu \left( 2\nu \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} \right) \frac{\varepsilon}{k} \quad (2.42)
\]

The new term in Chen's \( \varepsilon \) equation is \( C_{c3} \nu \frac{\varepsilon}{k} \), where \( P \) (2.37) is rewritten using the Boussinesq assumption (2.28). Chen's \( \varepsilon \) equation is hereby stronger tied to the production of \( k \), thereby giving it a response to changes in \( k \) at the same time as the changes are taking effect in \( k \). The coefficients of the models are tuned to experimental data and presented in table 2.1.

<table>
<thead>
<tr>
<th></th>
<th>( C_\mu )</th>
<th>( \sigma_k )</th>
<th>( \sigma_\varepsilon )</th>
<th>( C_{c1} )</th>
<th>( C_{c2} )</th>
<th>( C_{c3} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Launder and Spalding</td>
<td>0.09</td>
<td>1.0</td>
<td>1.22</td>
<td>1.44</td>
<td>1.92</td>
<td>0.25</td>
</tr>
<tr>
<td>Chen</td>
<td>0.09</td>
<td>0.75</td>
<td>1.15</td>
<td>1.15</td>
<td>1.9</td>
<td>0.25</td>
</tr>
</tbody>
</table>

2.7 Final form of the model equations for one-phase flow

The seven equations presented in this chapter form a closed set of equations that can be solved numerically, which describe highly turbulent Newtonian, incompressible, thermally variable, non-reactive, one-phase flow. They are the averaged continuity equation (2.20), the averaged Navier-Stokes equations (2.23), the averaged thermal energy equation (2.27), and the k-\( \varepsilon \) model equations (2.40-2.42). The modelling of the turbulent kinetic energy production term \( P \) (2.37) and the gradients in the Reynolds stresses and in the turbulent thermal energy fluxes with the Boussinesq assumption (2.28) and analog (2.32) is derived for incompressible flow in appendix B. The resulting terms are:

\[
\frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} = -\frac{\partial}{\partial x_j} \left( \nu \left( \frac{\partial \bar{u}_i}{\partial x_j} \right) \right) \quad (2.43)
\]
Table 2.2: The terms in the general equation for each flow-characteristic

<table>
<thead>
<tr>
<th>( \phi )</th>
<th>( \Gamma_\phi )</th>
<th>( S_\phi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( \mu + \mu_t )</td>
<td>( - \frac{\partial \rho}{\partial x_i} + \rho g_i )</td>
</tr>
<tr>
<td>( \bar{u}_i )</td>
<td>( \frac{\mu}{\sigma_k} )</td>
<td>( - \frac{\mu}{Pr_t} )</td>
</tr>
<tr>
<td>( \frac{\partial}{\partial x_i} ( \bar{u}_i \bar{u}_i + k ) )</td>
<td>( \frac{\mu}{\sigma_k} )</td>
<td>( \rho P - \rho \epsilon )</td>
</tr>
<tr>
<td>( \epsilon )</td>
<td>( \frac{\mu}{\sigma_\epsilon} )</td>
<td>( C_{e1} \frac{\rho \epsilon}{k} - C_{e2} \frac{\rho \epsilon^2}{k} + C_{e3} \frac{\mu_t P^2}{k} )</td>
</tr>
</tbody>
</table>

Where \( P = \nu_t \frac{\partial \bar{u}_i}{\partial x_i} \) and \( \mu_t = C_\mu \frac{k^2}{\epsilon} \).

Model equations for incompressible, non-reactive, Newtonian, one-phase turbulent flow with constant molecular viscosity \( \mu \). See table 2.1 for the values of the constants.

\[
\frac{\partial c_p T_{u_i}^j}{\partial x_i} = \frac{\partial}{\partial x_i} \left( - \frac{\nu_t}{Pr_t} \frac{\partial c_p T}{\partial x_i} \right) \quad (2.44)
\]

\[
P = \nu_t \frac{\partial u_j}{\partial x_i} \frac{\partial u_j}{\partial x_i} \quad (2.45)
\]

Now the seven equations can be put in the general form:

\[
\frac{\partial (\rho \phi)}{\partial t} = - \frac{\partial (u_j \rho \phi)}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \Gamma_\phi \frac{\partial \phi}{\partial x_j} \right) + S_\phi \quad (2.46)
\]

Where \( \rho \) is the constant density, \( u_j \) is an averaged velocity-component, \( x_j \) is the direction of the velocity-component, \( \Gamma_\phi \) is an effective gradient transport term for the scalar \( \phi \) and \( S_\phi \) is the source term for \( \phi \). The term on the left-hand-side represents the change in time of scalar \( \phi \), which is due to the terms on the right-hand-side, respectively due to convective transport, due to diffusive transport and due to source-terms. The terms for different \( \phi \)'s can be found in table 2.2.
Chapter 3

Particulate two-phase flow

Two-phase flow is a fluid motion of two phases, which are separated by an interfacial surface. These can be gas/solid (smoke), solid/liquid (quicksand), gas/liquid (rain or beer) or liquid/liquid (salad dressing: oil and vinegar). Particulate two-phase flow restricts one phase to a collection of particles dispersed in the other phase, the continuous carrier fluid. The particles interact with the carrier fluid by modulation of turbulence and by exchange of momentum, mass and energy. Depending on the volume fraction of the dispersed phase and the size of the particles, different interaction mechanisms have to be accounted for. The classification of two-phase flow on the basis of these interactions is presented in section 3.1.

The turbulent one-phase flow description presented in the previous chapter, can be classified as a model, due to the acceptance of the Boussinesq assumption, the k-ε models, the modelling of the molecular momentum transport with Newton’s Law of Viscosity and the molecular thermal energy transport with Fourier’s Law of Heat Conduction.

The turbulent particulate two-phase flow description is not yet in that stadium. The work done on the two-phase problem has resulted into two approaches. One approach is called Euler-Lagrangian, the other Euler-Euler. The Eulerian approach to the description of a phase is presented in chapter 2. The flow is taken as a continuum and the field is resolved on a fixed, three-dimensional grid. The values on the grid nodes represent the local averages of the continuous flow field. The Lagrangian approach to the description of a phase is to represent the phase by particles, where the history of the particle position, velocity and optionally other varying properties, such as temperature, diameter, density and component mass fractions are calculated based on the particle motion equations presented in section 3.2. Averaging these values around discrete positions in time and place, results in a flow field, which is the equivalent of the Eulerian flow field. The two approaches to the two-phase flow problem are presented in section 3.3. In that section derivations will be presented, from which the different formulations of two-phase flow in the literature can be analyzed. Because of the assumptions needed for the derivation, this analysis is restricted to non-rotating particles only.

The present state of the art is presented in the section on turbulence modulation, where the two approaches come together to formulate the terms needed to describe
Table 3.1: Coupling of dispersed two-phase flows as a function of particle volume fraction $\alpha_p$

<table>
<thead>
<tr>
<th>Coupling Type</th>
<th>$\alpha_p$ Condition</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>One-way coupling</td>
<td>$\alpha_p &lt; 10^{-6}$</td>
<td>Particle-motion is effected by the fluid motion: Turbulent dispersion.</td>
</tr>
<tr>
<td>Two-way coupling</td>
<td>$10^{-6} &lt; \alpha_p &lt; 10^{-3}$</td>
<td>Turbulence modulation by particles. Turbulent dispersion of particles</td>
</tr>
<tr>
<td>Four-way coupling</td>
<td>$\alpha_p &gt; 10^{-3}$</td>
<td>Next to the two-way coupling the particle-particle interaction is taken into account using collision models.</td>
</tr>
</tbody>
</table>

the effect of the presence of particles on turbulence.

3.1 Coupling in Two-Phase Flow

Dispersed two-phase flow is classified by Sommerfeld [9] with regard to the importance of interaction mechanisms (Table 3.1) into very dilute, dilute and dense flows. For very dilute flows (dispersed phase volume fraction $\alpha_p < 10^{-6}$) only the effect of the fluid motion on the particles is taken into account. This is called one-way coupling.

The dilute flow is characterized by two-way coupling. Here the particle presence affects the turbulence, which in turn disperses the particles. For dense dispersed two-phase flows ($\alpha_p > 10^{-3}$) the particle-particle interaction becomes important. Collisions models must be used and the average particle distance becomes a characteristic length for the turbulent flow, in addition to the Kolmogorov length-scale. Kenning and Crowe [22] propose a new hybrid length scale $l_h = (1/L_e + 1/\lambda)^{-1}$, composed of the integral length scale $L_e$ and the average particle distance $\lambda$ as a characterization of particulate multi-phase flow. $L_e$ is empirically determined to be one tenth of a pipe diameter and $\lambda \approx d_p[(\pi/6\alpha_d)^{1/3} - 1]$, where $d_p$ is the particle diameter and $\alpha_d$ is the dispersed phase volume fraction. The modulation predicted on the basis of this length scale agrees with experimental data, implying that the use of point particles, to simulate turbulence in fluid-particle systems will not capture the contribution due to inter-particle spacing. See also section 3.4. The coupling between particles and between particles and turbulent flow is called the four-way coupling problem and should not be considered completely solved.

3.2 Particle Motion Equations

Because the formulation of the Eulerian dispersed phase equations rely on the particle motion equations, these have to be presented first.
In Lagrangian analysis the particles, which form the dispersed phase, are usually not tracked individually, but are assumed to travel along the same trajectory with a number of other particles, in order to reduce the computational power needed. The trajectory is calculated for a particle, which represents the whole group: a parcel of particles. These parcels are treated as point-like, in the sense that their size and shape enter into the computation only via the semi-empirical drag coefficient. The tracking is done by solving the particle motion equation and the thermal energy equation. These equations, which account for the change in position, velocity and thermal energy, provide together with the parcel initial conditions a closed system for the modelling of trajectories. A trajectory is the collection of different positions in the fluid a parcel occupies before leaving the calculation domain. The equations for a particle with mass \( m_p \) for respectively position, velocity and thermal energy are:

\[
\frac{dx_{ip}}{dt} = v_{i,p} \tag{3.1}
\]

\[
m_p \frac{dv_{ip}}{dt} = \sum F_{i,r} \tag{3.2}
\]

\[
m_p \frac{d(c_{p,p}T_p)}{dt} = -A_{S,p}h(T_p - T_f) \tag{3.3}
\]

\( F_{i,r} \) represents the components of the different relevant forces acting on a particle. \( A_{S,p} \) is the particle surface area, \( c_{p,p} \) is the particle heat capacity, \( h \) is the heat transfer coefficient, \( T_p \) is the temperature of the particle and \( T_f \) is the local temperature of the fluid. The subscripts \( p \) and \( f \) refer respectively to the particle and the fluid phase. The heat coefficient is calculated using the Nusselt number:

\[
h = \frac{k_c Nu}{d_p} \tag{3.4}
\]

\[
Nu = 2(1 + 0.3Re_p^{1/2}Pr^{2/3}) \tag{3.5}
\]

\[
Re_p = \frac{\rho_f d_p |\bar{u}_f - \bar{v}_p|}{\mu_f} \tag{3.6}
\]

Where \( k_c \) is the thermal conductivity of the continuous phase, \( Nu \) is the Nusselt number, \( d_p \) is the particle diameter, \( Re_p \) is the particle Reynolds number, \( Pr \) is the Prandtl number and \( \mu_f \) is the fluid phase molecular viscosity.

### 3.2.1 Eddy life time model

To model the effect of turbulent dispersion on the particles the eddy life time model has been developed. (See also the section 3.3.2 on Eulerian Dispersed Phase Equations, especially equation 3.75.) In the eddy life time model turbulent flow is regarded as a collection of turbulent eddies with discrete velocities and life times. The fluid velocity encountered by the particle is constant during the time the particle remains in an eddy. The fluid velocity \( u_{i,f} \) is taken as the sum of the local time averaged fluid velocity \( \bar{u}_{i,f} \) and a fluctuating velocity \( u'_{i,f} \) selected from a Gaussian distribution with a variance proportional to the turbulence kinetic energy \( \sigma^2 = \frac{2k}{3} \).
An Euler-Lagrange analysis of turbulent two-phase mixing in a vertical pipe in a Star-CD environment

by Mark Moonen

Technische Universität Berlin
Institut für Verfahrenstechnik
Supervisor: Prof. Dr.-Ing. M. Kraume
Dr. Anja Paschedag
Dr. Alberto Varone
Dipl.-Ing. Manfredi Signorino
Technische Universität Delft
Kramers Laboratorium voor Fysische Technologie
Supervisor: Prof. Dr. H. van den Akker
Dr. Jos Derksen
Berlin, March 2002 - Delft, May 2003
Summary

Within the framework of the European Union PRATSOLIS project, an analysis of turbulent two-phase mixing in a vertical pipe by the commercial CFD code Star-CD environment has been performed. The aim of this study was to assess whether and how simulations of pipe flow can be performed in Star-CD, to create a Star-CD mesh of the pipe-flow for one- and two-phase flow simulation and to analyze Signorino’s experimental results. On the basis of experimental results taken from literature, Star-CD has been validated. It performs well for one-phase flow, but not for dilute two-phase flow. The reason for this is that Star-CD does not take turbulence modulation into account, nor can Star-CD be modified to do so. Signorino’s one-phase experimental data have been qualitatively well simulated. The obstruction of the flow due to the measuring device and the absence of accurate inlet conditions, makes a quantitatively correct simulation infeasible.
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Chapter 1

Introduction

1.1 PRATSOLIS

This thesis is a report of the work done between March 2002 and January 2003 at the TU Berlin and TU Delft, within the frame of the PRATSOLIS project. The acronym PRATSOLIS stands for PRecipitation and Agglomeration in Turbulent SOLid Liquid Systems and is a project with the aim to contribute to the development and implementation of models that can be integrated in computational fluid dynamics (CFD) codes and permit the prediction of precipitation and agglomeration in the typical complex systems which are met in industrial plants. The case of high solid volume fraction is particularly investigated.

Precipitation, also cited as reactive crystallization, consists in the mass crystallization of small solid particles by a phase transition from super-saturated solution to the solid phase. Agglomeration is the process of formation of one particle out of smaller particles.

The relevant point of the investigation of the PRATSOLIS-project to this study is the fluid-particle interaction. This point includes the analysis of what is usually called one-way, two-way and four-way interaction between particles and turbulence. One-way interaction points to the prevailing action of dispersion of particles exerted by the turbulent fluid on the particles. If the solid volume fraction is sufficiently high, the wakes generated by the particles modify the structure of turbulence and, in turn, affect the dispersion giving rise to two-way coupling. At even higher volume fractions, particle-particle collisions, particle-wall collisions and overlap of the wakes become important and modify further the turbulence structure, originating in four-way coupling. It should be noted that, although the interaction between fluid and particles is of hydrodynamic nature, it affects are those phenomena that are modulated by turbulence as, for instance, the rate of fast reactions, nucleation and growth of crystals, coagulation and breakage kinetics, and the resulting morphology of particles. More information about PRATSOLIS can be found at the web-site: http://www.esme.fr/pratsolis.
1.2 TU-Berlin Group

The group working on the PRATSOLIS project at the TU-Berlin consists of Manfredi Signorino, Alberto Varone, Anja Paschendag and Matthias Kraume. The experimental work of Signorino is focussed on the fluid-particle interaction for dense steady-state flows. He studies the effect of the addition of particles on the mixing of two in temperature differing water streams in a vertical downward pipe flow. Measurements of the radial temperature profiles at different axial positions at different volume fractions of particles are done intrusively using thermocouples, which are fixed at a radial position on a cross.

Simulations of one-phase and two-phase flow are performed, using the commercial CFD-code Star-CD. Star-CD developed a framework for dispersed multi-phase flow, such as can be found in liquid- and solid-fuelled combustors, spray driers, cyclone dust separators and chemical reactors. Mostly large scale equipment, in which the calculation of the particle trajectories is of main importance. In all cases the flow consists of a continuous phase and one or more dispersed phases in the form of particles. The motion of the dispersed phase will be effected by that of the continuous one and vice versa via displacement and inter-phase momentum, mass and heat transfer effects. The strength of the interactions will depend on the dispersed phase particle’s size, density and number density. Next to this Star-CD provides models for particle-particle collisions and particle-wall collisions.

The emphasis of the current work of the TU-Berlin group does not lay on the correct calculation of the particle trajectories, but on the effect of the particles on turbulence. Therefore Star-CD will have to be tested and possibly adapted to calculate this effect correctly.

1.3 The aim of this study

The aim of this study is to support Signorino’s experimental work by simulation in the Star-CD environment: to assess whether and how two-phase simulations of the pipe flow can be performed in Star-CD, to create a Star-CD mesh of the pipe-flow for one- and two-phase flow simulation and to analyze Signorino’s experimental results.

1.4 Setup of the thesis

Two-phase turbulent flow description relies heavily on one-phase turbulent flow description. Therefore one-phase turbulent flow is treated in chapter 2, followed by turbulent two-phase flow in chapter 3. To perform simulations with the model equations derived in chapter 2 and 3, they are converted into algebraic relations, which are solved in numerical algorithms. This is presented in chapter 4. In chapter 5 the implementation of multiphase turbulent flow in Star-CD is treated, with an emphasis on the differences with the model equations, algebraic relations and numerical algorithms presented in the previous three chapters. In chapter 6 the results are presented of the assessment of Star-CD two-phase simulation capabilities, of the
1.4. SETUP OF THE THESIS

mesh construction for two-phase flow and of the preliminary analysis of Signorino's experimental results. The conclusions are presented in chapter 7.
Chapter 2

One-Phase Flow

In the first section (2.1) some words will be spent on the phenomenon of turbulence and the basic quantification of turbulence in scales and dimensional quantities. Turbulent one-phase flow of an incompressible fluid can be described using a set of four equations: the continuity equation and the three Navier-Stokes equations. For the description of the temperature field the thermal energy equation is used. They will be derived in section 2.2.

However, the flow field can not be resolved down to the smallest scale of turbulence for highly turbulent flows. Therefore the equations will have to be transformed into their averaged counterparts (section 2.3). This gives rise to averaged products of fluctuations. These new terms are the Reynolds stresses and the turbulent scalar fluxes.

These can be modelled using the Boussinesq assumption and analogs (section 2.4). The turbulent viscosity, which is introduced in the Boussinesq assumption can be calculated from the turbulent kinetic energy $k$ and the turbulent energy dissipation $\epsilon$. An equation to describe the turbulent kinetic energy, including the definition of $\epsilon$, is derived in section 2.5. In section 2.6 the standard $k$-$\epsilon$ model and Chen’s $k$-$\epsilon$ model are presented.

The averaged continuity, averaged Navier-Stokes, averaged thermal energy and the $k$-$\epsilon$ model form a closed set of equations that can be solved numerically, which describe one-phase, thermally varying, non-reactive flow. They are summarized and put into general form in section 2.7.

2.1 Turbulence Description

A basic distinction in fluid dynamics is the distinction between laminar and turbulent flow. In laminar flow the flow can be thought of as a collection of laminae, where each lamina slides with constant velocity between two other laminae. In a confined flow such as pipe flow a laminar flow can be realized, when the throughput is low enough. At the wall the cylindrical fluid lamina has no velocity, while the center lamina has the maximum velocity. Due to friction between the laminae, the resulting velocity profile in the radial direction is parabolic.

When the throughput $\varphi_\nu$ is increased, there will be a point at which the friction
can no longer level the velocity gradient and turbulence kicks in. The flow stumbles over slower parts of the fluid, creating non-laminar motion. The Reynolds number is defined as:

\[ Re = \frac{\rho UD}{\mu} \]  

(2.1)

where \( D \) is the pipe diameter, \( \rho \) is the fluid density, \( \mu \) is the fluid viscosity and \( U = \phi_0/(\pi/4 D^2) \) is the superficial velocity. The magnitude of this dimensionless group gives an indication of the relative importance of inertial and viscous fluid forces. When the viscous fluid force dominates the flow is laminar, when the inertial force is dominant the flow is turbulent. Pipe flow is fully turbulent for \( Re > 2.1 \cdot 10^4 \) [1].

When laminar pipe flow can be characterized by fluid cylinders sliding at constant speed in and over other cylinders, turbulent flow is characterized by eddy structures. An eddy is a swirling motion through the flow. Due to their motion they produce eddies of a smaller scale, which in turn produce smaller scaled eddies, down to a scale at which the velocity gradient is small enough to be handled by molecular viscosity.

Thus in the turbulent regime kinetic energy is transferred to turbulent kinetic energy \( k \) in the form of circulatory motion. The turbulent kinetic energy \( k \) flows down a cascade of ever in size decreasing eddies, until an eddy size at which the molecular dissipation can catch up again. In steady-state the rate of kinetic energy \( k \) flowing down this cascade is equal to the turbulent energy dissipation \( \epsilon \).

Dimensional analysis led Kolmogorov [2] to the definition of the time scale \( t_K \), the length scale \( l_K \) and the velocity scale \( u_K \) of the smallest eddies:

\[ t_K = \left( \frac{\nu}{\epsilon} \right)^{1/2} \]  

(2.2)

\[ l_K = \left( \frac{\nu^3}{\epsilon} \right)^{1/4} \]  

(2.3)

\[ u_K = (\nu \epsilon)^{1/4} \]  

(2.4)

Where \( \nu = \mu/\rho \) is the kinematic viscosity, \( \mu \) is the molecular viscosity and \( \rho \) is the fluid density. Defining a smallest eddy Reynolds number as

\[ Re_K = \frac{u_K l_K}{\nu} = 1, \]

shows the flow of the smallest eddy to be truly laminar, being viscously dissipated in a time \( t_K \).

Contrary to laminar flow, the velocity at one point is not constant. Depending on the passage of an eddy, the velocity at a point is a random variable. Because of this chaotic nature of turbulence it is not possible to predict the instantaneous velocity of a particular flow. Turbulence description is therefore stochastic and deals with averages and variations around averages.
2.2. MASS, MOMENTUM AND THERMAL ENERGY BALANCES OVER A BOX

2.2.1 Turbulence Description with numerical simulations

In computational fluid dynamics (CFD) the flow field is taken as space and time dependent changing of variables governed by conservation equations. These equations will be derived in the following sections. Space and time are discretized into finite elements, giving rise to a grid. By solving the governing equations together with the boundary conditions, particular to a certain flow, the flow field can be calculated. This type of computation is called Direct Numerical Simulation (DNS) and is computationally quite intensive. At the present it is only possible for relatively low Reynolds numbers, because DNS has to resolve down to the scales of the smallest eddies. These scales decrease with increasing turbulence, demanding more computing power, thereby limiting the application of DNS.

To describe stronger turbulent flows, time and space are discretized into elements larger than the Kolmogorov scales. This means that the Navier-Stokes equations, which will be derived in section 2.2, cannot be used, because they refer to a point in the flow. When the flow is resolved beyond the smallest structure, they can be resolved numerically, but another set of equations is needed for coarser grids. This set is generated by averaging the Navier-Stokes equations. However the averaged variables are influenced by the effect of the fluctuations from average. This effect has to be accounted for. An example of fluctuations, which have an effect on the averaged variables, are the Reynolds stresses. The Reynolds stresses account for the turbulent momentum transport, due to the velocity fluctuations. The modelling of the Reynolds stresses by averaged strains on the finite grid elements is treated in section 2.4. With the modelling of the averaged products of fluctuations two other scalars are introduced: the turbulent kinetic energy $k$ and its dissipation $\epsilon$. Next to the continuity, the three velocity component and the thermal energy transport equations, two other transport equations will be needed for the new scalars. Sections 2.5 and 2.6 treat the derivation of these equations of change.

When the turbulent flow field has (locally) in every direction the same turbulent characteristics, it is called (locally) isotropic. Isotropic turbulence is invariant to the interchanging of the space-directions, allowing a simplification of the description. When the turbulent flow field has the same characteristics over a spatial distance, it is called homogeneous turbulence. This allows the use of finite volumes for the description of the space dependence of the flow field.

2.2 Mass, Momentum and Thermal Energy Balances over a Box

In this section the continuity, the Navier-Stokes equations and the change of thermal energy will be derived by writing the mass, momentum and thermal energy balances over a box.

Over a box of finite dimensions $\Delta x$, $\Delta y$, $\Delta z$ at $x$, $y$, $z$ the mass balance is:

$$\text{change of mass} = \text{mass flow}_{\text{in}} - \text{mass flow}_{\text{out}}$$
CHAPTER 2. ONE-PHASE FLOW

\[
\frac{\Delta \rho (\rho \Delta x \Delta y \Delta z)}{\Delta t} = u_x \rho \Delta y \Delta z \bigg|_x - u_x \rho \Delta y \Delta z \bigg|_{x+\Delta x} + \\
+ u_y \rho \Delta x \Delta z \bigg|_y - u_y \rho \Delta x \Delta z \bigg|_{y+\Delta y} + \\
+ u_z \rho \Delta x \Delta y \bigg|_z - u_z \rho \Delta x \Delta y \bigg|_{z+\Delta z}
\] (2.5)

Where \( \rho \) is the fluid density and \( u_x, u_y, u_z \) are the velocity components in respectively the x, y and z direction.

Shrinking the dimensions of the box and the time of change to almost zero, using \( \frac{\partial f}{\partial x} = \lim_{\Delta x \to 0} \frac{f(x+\Delta x)-f(x)}{\Delta x} \) and rearranging, this becomes:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_x)}{\partial x} + \frac{\partial (\rho u_y)}{\partial y} + \frac{\partial (\rho u_z)}{\partial z} = 0
\] (2.6)

Using the Einstein convention:

\[
\frac{\partial u_i}{\partial x_i} = \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z}
\] (2.7)

where \( i, j = 1, 2, 3 \) and \( x_1 = x, x_2 = y, x_3 = z \), gives the continuity-equation:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0
\] (2.8)

If the flow is incompressible, as can be assumed for a liquid, \( \rho = \text{constant} \). This reduces the continuity equation for incompressible flow to:

\[
\frac{\partial u_i}{\partial x_i} = 0
\] (2.9)

The incompressible continuity equation couples gradients of the different velocity-components and is used in the derivation of the Navier-Stokes equation.

Over a box of finite dimensions \( \Delta x \Delta y \Delta z \) at \( x, y, z \) the x-momentum-balance is:

\[
\text{change of momentum}_x = \text{momentum}_x \text{flow}_{\text{in}} - \text{momentum}_x \text{flow}_{\text{out}} + \text{forces}_x
\]

The forces considered are pressure, gravity and friction.

\[
\frac{\Delta (\rho u_x \Delta x \Delta y \Delta z)}{\Delta t} = u_x u_x \rho \Delta y \Delta z \bigg|_x - u_x u_x \rho \Delta y \Delta z \bigg|_{x+\Delta x} + \\
+ u_y u_x \rho \Delta x \Delta z \bigg|_y - u_y u_x \rho \Delta x \Delta z \bigg|_{y+\Delta y} + \\
+ u_z u_x \rho \Delta x \Delta y \bigg|_z - u_z u_x \rho \Delta x \Delta y \bigg|_{z+\Delta z}
\]
2.2. MASS, MOMENTUM AND THERMAL ENERGY BALANCES OVER A BOX

\[ +u_xu_z\rho \Delta x \Delta y \bigg|_{x} - u_xu_z\rho \Delta x \Delta y \bigg|_{x+\Delta x} \]
\[ +\tau_{xx}\Delta y \Delta z \bigg|_{x} - \tau_{xx}\Delta y \Delta z \bigg|_{x+\Delta x} \]
\[ +\tau_{yx}\Delta x \Delta z \bigg|_{y} - \tau_{yx}\Delta x \Delta z \bigg|_{y+\Delta y} \]
\[ +\tau_{zz}\Delta x \Delta y \bigg|_{z} - \tau_{zz}\Delta x \Delta y \bigg|_{z+\Delta z} \]
\[ +p_x\Delta y \Delta z \bigg|_{z} - p_x\Delta y \Delta z \bigg|_{z+\Delta z} \]
\[ +\rho g_x \Delta x \Delta y \Delta z \]  (2.10)

With the dimensions of the box and the change of time approaching zero and rearranging, gives:

\[
\frac{\partial (p u_x)}{\partial t} = -\frac{\partial (p u_x u_x)}{\partial x} - \frac{\partial (p u_y u_x)}{\partial y} - \frac{\partial (p u_z u_x)}{\partial z} + \\
-\frac{\partial \tau_{xx}}{\partial x} - \frac{\partial \tau_{yx}}{\partial y} - \frac{\partial \tau_{zx}}{\partial z} + \\
-\frac{\partial p}{\partial x} + \rho g_x \]  (2.11)

Using suffix-notation this can be generalized to the Navier-Stokes equation for compressible flow:

\[
\frac{\partial (\rho u_i)}{\partial t} = -\frac{\partial (\rho u_j u_i)}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial p}{\partial x_i} + \rho g_i \]  (2.12)

Assuming the fluid is Newtonian, the stress tensor is linearly dependent on the velocity gradient. Using Newton's law of viscosity [1]: \( \tau_{ij} = -\mu \frac{\partial u_i}{\partial x_j} \), assuming \( \rho = \text{constant} \) and rearranging using the continuity equation 2.9, gives the Navier-Stokes equation for single-phase constant density flows:

\[
\frac{\partial u_i}{\partial t} = -u_j \frac{\partial u_i}{\partial x_j} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} - \frac{1}{\rho} \frac{\partial p}{\partial x_i} + g_i \]  (2.13)

The first term on the right-hand-side of the equation represents the change of the velocity-component due to convective momentum transport, the second due to molecular transport of momentum and the third and fourth due to the pressure-gradient and gravity.

Over a box of finite dimensions \( \Delta x \Delta y \Delta z \) at \( x, y, z \) the thermal energy balance for incompressible flow is:

\[
\text{change of thermal energy} = \text{thermal energy flow in} + \\
- \text{thermal energy flow out} + \\
+ \text{thermal energy produced by friction} \]
The energy flux is divided into convection and conduction. The convective flux is due to the fluid motion, the conductive flux $q_i$ is due to a thermal energy gradient. The kinetic energy loss due to the levelling of velocity differences by friction is equal to the thermal energy production.

\[
\Delta(c_p T \rho \Delta x \Delta y \Delta z) \over \Delta t = \left. c_p T u_x \rho \Delta y \Delta z \right|_x - \left. c_p T u_x \rho \Delta y \Delta z \right|_{x+\Delta x} + \\
+ \left. c_p T u_y \rho \Delta x \Delta z \right|_y - \left. c_p T u_y \rho \Delta x \Delta z \right|_{y+\Delta y} + \\
+ \left. c_p T u_z \rho \Delta x \Delta y \right|_z - \left. c_p T u_z \rho \Delta x \Delta y \right|_{z+\Delta z} + \\
+ q_x \Delta y \Delta z |_x - q_x \Delta y \Delta z |_{x+\Delta x} + q_y \Delta x \Delta z |_y + \\
- q_y \Delta x \Delta z |_{y+\Delta y} + q_z \Delta x \Delta y |_z - q_z \Delta x \Delta y |_{z+\Delta z} + \\
- (u_x \tau_{xx} + u_y \tau_{yx} + u_z \tau_{xz}) \Delta y \Delta z |_x + \\
+ (u_x \tau_{xx} + u_y \tau_{yx} + u_z \tau_{xz}) \Delta y \Delta z |_{x+\Delta x} + \\
- (u_x \tau_{xy} + u_y \tau_{yy} + u_z \tau_{yz}) \Delta x \Delta z |_y + \\
+ (u_x \tau_{xy} + u_y \tau_{yy} + u_z \tau_{yz}) \Delta x \Delta z |_{y+\Delta y} + \\
- (u_x \tau_{xz} + u_y \tau_{yz} + u_z \tau_{zz}) \Delta x \Delta y |_z + \\
+ (u_x \tau_{xz} + u_y \tau_{yz} + u_z \tau_{zz}) \Delta x \Delta y |_{z+\Delta z} \tag{2.14}
\]

With the dimensions of the box and the change of time approaching zero, constant density $\rho$ and rearranging, gives:

\[
\frac{\partial (c_p T)}{\partial t} = -u_x \frac{\partial (c_p T)}{\partial x} - u_y \frac{\partial (c_p T)}{\partial y} - u_z \frac{\partial (c_p T)}{\partial z} + \\
- \frac{1}{\rho} \frac{\partial q_x}{\partial x} - \frac{1}{\rho} \frac{\partial q_y}{\partial y} - \frac{1}{\rho} \frac{\partial q_z}{\partial z} + \\
+ \frac{1}{\rho} \frac{\partial (u_x \tau_{xx} + u_y \tau_{yx} + u_z \tau_{xz})}{\partial x} + \\
+ \frac{1}{\rho} \frac{\partial (u_x \tau_{xy} + u_y \tau_{yy} + u_z \tau_{yz})}{\partial y} + \\
+ \frac{1}{\rho} \frac{\partial (u_x \tau_{xz} + u_y \tau_{yz} + u_z \tau_{zz})}{\partial z} \tag{2.15}
\]

Using Fourier's Law of Heat Conduction [1]: $q_i = -\lambda \frac{\partial (c_p T)}{\partial x_i}$ and rearranging, gives
2.3. VARIABLE AVERAGING OVER TIME OR VOLUME

the equation of change of thermal energy:

$$\frac{\partial (c_p T)}{\partial t} = -\frac{u_i}{\rho} \frac{\partial (c_p T)}{\partial x_i} + \lambda \frac{\partial^2 (c_p T)}{\partial x_i \partial x_i} + \frac{1}{\rho} \frac{\partial (u_i \tau_{ij})}{\partial x_j}$$  \hspace{1cm} (2.16)

Rewriting this equation using Newton’s Law of viscosity: \(\tau_{i,j} = -\mu \frac{\partial u_j}{\partial x_i}\), reveals the thermal energy source term as the result from the change of kinetic energy due to friction:

$$\frac{\partial (c_p T)}{\partial t} = -\frac{u_i}{\rho} \frac{\partial (c_p T)}{\partial x_i} + \lambda \frac{\partial^2 (c_p T)}{\partial x_i \partial x_i} - \nu \frac{\partial^2 (u_i u_j)}{\partial x_j \partial x_j}$$  \hspace{1cm} (2.17)

2.3 Variable Averaging over Time or Volume

As mentioned in section 2.1 CFD makes use of grid-averaged variables, which equations contain the effect of fluctuations on the grid-averaged variables. The continuity, Navier-Stokes and thermal energy equations are derived for control volumes approaching zero volume, i.e. points in the flow field. So the point equations will be averaged over a finite time or over a finite volume, resulting in averaged flow-field properties such as the averaged velocity-components \(\overline{u_i}\) and the averaged thermal energy \(\overline{c_p T}\).

The local velocity can be decomposed in the average velocity and a velocity fluctuation due to the presence of eddies. For time this is known as Reynolds decomposition, more generally put

$$X = \overline{X} + X', \quad \overline{X} = \overline{X} + X' = \overline{X} + \overline{X'} \quad \text{thus} \quad \overline{X'} = 0$$  \hspace{1cm} (2.18)

More general is the following formulation:

$$\left< X \right> = \frac{1}{Y} \int_0^Y X \, dY = \frac{1}{Y} \int_0^Y \left( \left< X \right> + X' \right) \, dY = \left< X \right> + \frac{1}{Y} \int_0^Y X' \, dY \quad \text{thus} \quad \left< X' \right> = 0$$  \hspace{1cm} (2.19)

Where Y is a finite time or volume. In this thesis Reynolds notation will be used, with the remark that in all equations it can be interchanged with the more general notation.

For turbulent flow it is necessary to average the continuity equation 2.9, the Navier-Stokes equation 2.13 and the thermal equation 2.17. The averaged continuity equation becomes:

$$\overline{\frac{\partial (\overline{u_i} + u'_i)}{\partial x_i}} = \frac{\partial \overline{u_i}}{\partial x_i} = 0$$  \hspace{1cm} (2.20)

Averaging of the Navier-Stokes equation (2.13):

$$\overline{\frac{\partial (\overline{u_i} + u'_i)}{\partial t}} = -\left(\overline{u_j} + u'_j\right) \frac{\overline{\partial (\overline{u_i} + u'_i)}}{\partial x_j} + \nu \frac{\partial^2 (\overline{u_i} + u'_i)}{\partial x_j \partial x_j}$$

$$+ \frac{1}{\rho} \frac{\partial (\overline{p + y'})}{\partial x_i} + \frac{g_i}{\rho}$$  \hspace{1cm} (2.21)
The averaging of the transport terms gives rise to the Reynolds-stresses:

$$
(u_j + u'_j) \frac{\partial (\bar{u}_j + u'_j)}{\partial x_j} = \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} + u'_j \frac{\partial u'_i}{\partial x_j} = \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial (u'_j u'_i)}{\partial x_j} - u'_i \frac{\partial u'_j}{\partial x_j} = 0 \tag{2.22}
$$

Resulting in the Reynolds-averaged Navier-Stokes (RANS) equation:

$$
\frac{\partial \bar{u}_i}{\partial t} = -\bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_i \partial x_j} - \frac{1}{\rho} \frac{\partial p}{\partial x_i} + g_i - \frac{\partial u'_i u'_j}{\partial x_j} \tag{2.23}
$$

Averaging the thermal energy equation (2.17):

$$
\frac{\partial (c_p(T + T'))}{\partial t} = -\frac{(u_i + u'_i)}{\partial x_i} \frac{\partial (c_p(T + T'))}{\partial x_i} + \frac{\lambda}{\rho} \frac{\partial^2 (c_p(T + T'))}{\partial x_i \partial x_i} + \nu \frac{\partial^2 (\frac{1}{2} (u_i + u'_i)^2)}{\partial x_j \partial x_j} \tag{2.24}
$$

The averaging of transport terms is analogue to 2.22, gives rise to the turbulent thermal energy fluxes:

$$
(u_i + u'_i) \frac{\partial (c_p(T + T'))}{\partial x_i} = \bar{u}_i \frac{\partial c_p \bar{T}}{\partial x_i} + \frac{\partial c_p T' u'_i}{\partial x_i} \tag{2.25}
$$

And even more terms arise by averaging the thermal energy production term:

$$
\nu \frac{\partial^2 (\frac{1}{2} (u_i + u'_i)^2)}{\partial x_j \partial x_j} = \nu \frac{\partial^2 (\frac{1}{2} \bar{u}_i^2)}{\partial x_j \partial x_j} + \nu \frac{\partial^2 (\frac{1}{2} u'_i u'_j)}{\partial x_j \partial x_j} \tag{2.26}
$$

Resulting in the averaged thermal energy equation:

$$
\frac{\partial c_p \bar{T}}{\partial t} = -\bar{u}_i \frac{\partial c_p \bar{T}}{\partial x_i} + \frac{\lambda}{\rho} \frac{\partial^2 c_p \bar{T}}{\partial x_i \partial x_i} - \nu \frac{\partial^2 (\frac{1}{2} \bar{u}_i \bar{u}_i)}{\partial x_j \partial x_j} + \frac{\partial c_p T' u'_i}{\partial x_i} - \nu \frac{\partial^2 (\frac{1}{2} u'_i u'_j)}{\partial x_j \partial x_j} \tag{2.27}
$$
2.4 The Boussinesq Assumption

After averaging the Navier-Stokes and the thermal energy equation some terms remain unclosed. The Reynolds stresses \( \overline{u_i'u_j} \) and the turbulent thermal energy fluxes \( c_p T' u'_i \) need modeling as mentioned before, thereby closing the system of equations. The Boussinesq assumption for \( \rho \) constant is:

\[
\overline{u_i'u_j} = -2\nu_s \delta_{ij} + \frac{2}{3} k \delta_{ij}
\]

(2.28)

Where \( \delta_{ij} \) is the Kronecker delta:

\[
\delta_{ij} = \begin{cases} 
1 & \text{if } i=j \\
0 & \text{if } i\neq j,
\end{cases}
\]

(2.29)

\( \delta_{ij} \) represents the average strain terms:

\[
\delta_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)
\]

(2.30)

and \( \nu_t \) the turbulent kinematic viscosity:

\[
\nu_t \equiv C_\mu \frac{k^2}{\epsilon} \quad \text{where} \quad C_\mu = 0.09 \quad [3]
\]

(2.31)

Where \( k \) and \( \epsilon \) are respectively the turbulent kinetic energy and its dissipation rate. They will be treated in the sections 2.5 and 2.6. The turbulent viscosity \( \mu_t = \rho \nu_t \) introduced with the Boussinesq assumption, gives in analogy to the molecular viscosity \( \mu \) the turbulent fluxes as the product of a 'constant' and a gradient. In analogy to the Boussinesq assumption the turbulent thermal energy fluxes are:

\[
c_p T' u'_i = -\frac{\nu_t}{Pr_t} \frac{\partial c_p T}{\partial x_i}
\]

(2.32)

Where \( Pr_t \) is the turbulent Prandtl number.

The modeling of the Reynolds stresses and turbulent scalar fluxes moves the closure problem to \( k \) and \( \epsilon \). In the next section the \( k \) equation will be presented.

2.5 Turbulent Kinetic Energy, the \( k \)-equation.

The turbulent kinetic energy, i.e. energy contained in eddy motion, has a mass concentration of \( k \):

\[
k \equiv \frac{1}{2} (u'_x u'_x + u'_y u'_y + u'_z u'_z) = \frac{1}{2} \overline{u_i'u_i}
\]

(2.33)

The change in \( k \) can be rewritten as:

\[
\frac{\partial k}{\partial t} = \frac{\partial}{\partial t} \left( \frac{1}{2} \overline{u_i'u_i} \right) = \frac{\partial u'_i}{\partial t} \frac{\partial u'_i}{\partial t} = u'_i \left( \frac{\partial u_i}{\partial t} - \frac{\partial u_i}{\partial t} \right)
\]

(2.34)
So to derive the $k$ equation, the manipulations of the Navier-Stokes equation (2.13) that are needed, are subsequently averaging of the Navier-Stokes equation, (resulting in 2.23,) deduction of the averaged equation from the Navier-Stokes equation, multiplication of the difference with the velocity fluctuation and finally averaging of the product. The derivation of the $k$-equation is presented in appendix A. The $k$-equation, which is identical to equation 5.132 of Pope [4], is:

\[
\frac{\partial k}{\partial t} = -\overline{u_j} \frac{\partial k}{\partial x_j} - \frac{\partial}{\partial x_j} T_j + P - \epsilon \tag{2.35}
\]

where

\[
T_j = \frac{1}{2} u_i' u_j' + \frac{\overline{\nu_i' u_j'}}{\rho} - 2 \nu \overline{u_i s'_{ij}} \tag{2.36}
\]

\[
P = -\overline{u_i' u_j'} \overline{\partial u_i \overline{\partial x_j}} \tag{2.37}
\]

\[
\epsilon = 2 \nu s'_{ij} s'_{ij} \tag{2.38}
\]

\[
s'_{ij} = \frac{1}{2} \left( \frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i} \right) \tag{2.39}
\]

The first term on the right-hand side of 2.35 represents the scalar transport due to convection, the second term is transport due to turbulent scalar fluxes, $P$ is the turbulent energy production, $\epsilon$ is the turbulent energy dissipation and $s'_{ij}$ used in the definition of $\epsilon$ represent the fluctuations of the strain at a point.

### 2.6 The $k/\epsilon$-equations

Moving the closure problem introduced with the Reynolds stresses and the turbulent scalar fluxes to the turbulent viscosity, which is evaluated with $k$ and $\epsilon$, shifts the problem to two other terms involving averaged products of fluctuations: $\epsilon$ and $T_j$. These terms can be evaluated by solving a transport equation for them, or by modelling. Launder and Spalding [3] represent all third order correlation which appear in the $k$ equation (2.35) 'in absence of superior knowledge' by way of gradients of $k$. Thus

\[
\frac{\partial T_j}{\partial x_j} = \frac{\partial}{\partial x_j} \left( D_k \frac{\partial k}{\partial x_j} \right)
\]

where $D_k$ is an effective diffusion coefficient for the turbulence energy $k$, depending on the turbulence regime. They solve a transport equation for $\epsilon$. At high Reynolds numbers the transport equations for $k$ and $\epsilon$ may be expressed:

\[
\frac{\partial k}{\partial t} = -\overline{u_j} \frac{\partial k}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \frac{\nu_t}{\sigma_k} \frac{\partial k}{\partial x_j} \right) + 2 \nu \overline{s_{ij} \partial u_i \overline{\partial x_j}} - \epsilon \tag{2.40}
\]

\[
\frac{\partial \epsilon}{\partial t} = -\overline{u_j} \frac{\partial \epsilon}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \frac{\nu_t}{\sigma_{\epsilon}} \frac{\partial \epsilon}{\partial x_j} \right) + \\
+ C_{\epsilon 1} \frac{\epsilon}{k} (2 \nu \overline{s_{ij} \partial u_i \overline{\partial x_j}} - C_{\epsilon 2} \frac{\epsilon^2}{k}) \tag{2.41}
\]
2.7. FINAL FORM OF THE MODEL EQUATIONS FOR ONE-PHASE FLOW

Originally assessed by Launder and Spalding [3] for free turbulent flow the k-\(\epsilon\) model could not represent some turbulent flow problems. The spreading rate of a round jet is over-predicted by more than 30% and for the turbulent flow over a backwards facing step the re-attachment length is under-predicted by more than 25%. Because the dissipation rate equation is highly empirical in nature, improvement of the model performance is usually achieved by modifying the dissipation rate equation. Chen [5] introduced an additional term in the \(\epsilon\)-equation to add a second time scale of the production range of the turbulent kinetic energy spectrum. Hereby enabling the energy transfer mechanism of the turbulence model to respond to the mean strain more effectively.

\[
\frac{\partial \epsilon}{\partial t} = -\overline{u_j \partial \epsilon}  + \frac{\partial}{\partial x_j} \left( \frac{\nu_t \partial \epsilon}{\sigma_\epsilon \partial x_j} \right) + C_{\epsilon 1} \frac{\epsilon}{k} \left( 2\nu_t \overline{\omega_i \partial u_i} \right) + \\
- C_{\epsilon 2} \frac{\epsilon^2}{k} + C_{\epsilon 3} \nu_t \left( 2\nu_t \overline{\omega_i \partial u_i} \right)^2 \frac{1}{k} 
\]

(2.42)

The new term in Chen’s \(\epsilon\) equation is \(C_{\epsilon 3} \nu_t P^2 / k\), where \(P\) (2.37) is rewritten using the Boussinesq assumption (2.28). Chen’s \(\epsilon\) equation is hereby stronger tied to the production of \(k\), thereby giving it a response to changes in \(k\) at the same time as the changes are taking effect in \(k\). The coefficients of the models are tuned to experimental data and presented in table 2.1.

<table>
<thead>
<tr>
<th></th>
<th>(C_n)</th>
<th>(\sigma_k)</th>
<th>(\sigma_\epsilon)</th>
<th>(C_{\epsilon 1})</th>
<th>(C_{\epsilon 2})</th>
<th>(C_{\epsilon 3})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Launder and Spalding</td>
<td>0.09</td>
<td>1.0</td>
<td>1.22</td>
<td>1.44</td>
<td>1.92</td>
<td>0.25</td>
</tr>
<tr>
<td>Chen</td>
<td>0.09</td>
<td>0.75</td>
<td>1.15</td>
<td>1.15</td>
<td>1.9</td>
<td>0.25</td>
</tr>
</tbody>
</table>

2.7 Final form of the model equations for one-phase flow

The seven equations presented in this chapter form a closed set of equations that can be solved numerically, which describe highly turbulent Newtonian, incompressible, thermally variable, non-reactive, one-phase flow. They are the averaged continuity equation (2.20), the averaged Navier-Stokes equations (2.23), the averaged thermal energy equation (2.27), and the k-\(\epsilon\) model equations (2.40-2.42). The modelling of the turbulent kinetic energy production term \(P\) (2.37) and the gradients in the Reynolds stresses and in the turbulent thermal energy fluxes with the Boussinesq assumption (2.28) and analog (2.32) is derived for incompressible flow in appendix B. The resulting terms are:

\[
\frac{\partial \overline{u_i' u_j'}}{\partial x_j} = - \frac{\partial}{\partial x_j} \left( \nu_t \left( \frac{\partial \overline{u_i}}{\partial x_j} \right) \right) 
\]

(2.43)
Table 2.2: The terms in the general equation for each flow-characteristic

<table>
<thead>
<tr>
<th>( \phi )</th>
<th>( \Gamma_{\phi} )</th>
<th>( S_{\phi} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( \mu + \mu_t )</td>
<td>( - \frac{\partial P}{\partial x_i} + \rho g_i )</td>
</tr>
<tr>
<td>( u_i )</td>
<td>( \frac{\mu}{c_p P_r} + \frac{\mu_t}{P_r} )</td>
<td>( -\mu \frac{\partial^2 (\frac{1}{2} \overline{u_i} \overline{u_i} + k)}{\partial x_j \partial x_j} )</td>
</tr>
<tr>
<td>( k )</td>
<td>( \frac{\mu_t}{\sigma_k} )</td>
<td>( \rho P - \rho \varepsilon )</td>
</tr>
<tr>
<td>( \epsilon )</td>
<td>( \frac{\mu_t}{\sigma_\epsilon} )</td>
<td>( C_{\epsilon 1} \frac{\rho \varepsilon}{k} P - C_{\epsilon 2} \frac{\rho \varepsilon^2}{k} + C_{\epsilon 3} \frac{\mu_t P^2}{k} )</td>
</tr>
</tbody>
</table>

Where \( P = \nu_t \frac{\partial \overline{u_i} \partial \overline{u_i}}{\partial x_i \partial x_i} \) and \( \mu_t = C_{\mu} \frac{k^2}{\epsilon} \).

Model equations for incompressible, non-reactive, Newtonian, one-phase turbulent flow with constant molecular viscosity \( \mu \). See table 2.1 for the values of the constants.

\[
\frac{\partial c_p T' u'_i}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \frac{\nu_t}{P_{r_t}} \frac{\partial c_p T'}{\partial x_i} \right) \tag{2.44}
\]

\[
P = \nu_t \frac{\partial \overline{u_j} \partial \overline{u_i}}{\partial x_i \partial x_i} \tag{2.45}
\]

Now the seven equations can be put in the general form:

\[
\frac{\partial (\rho \phi)}{\partial t} = - \frac{\partial (\overline{u_j} \rho \phi)}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \Gamma_{\phi} \frac{\partial \phi}{\partial x_j} \right) + S_{\phi} \tag{2.46}
\]

Where \( \rho \) is the constant density, \( \overline{u_j} \) is an averaged velocity-component, \( x_j \) is the direction of the velocity-component, \( \Gamma_{\phi} \) is an effective gradient transport term for the scalar \( \phi \) and \( S_{\phi} \) is the source term for \( \phi \). The term on the left-hand-side represents the change in time of scalar \( \phi \), which is due to the terms on the right-hand-side, respectively due to convective transport, due to diffusive transport and due to source-terms. The terms for different \( \phi \)'s can be found in table 2.2.
Chapter 3

Particulate two-phase flow

Two-phase flow is a fluid motion of two phases, which are separated by an interfacial surface. These can be gas/solid (smoke), solid/liquid (quicksand), gas/liquid (rain or beer) or liquid/liquid (salad dressing: oil and vinegar). Particulate two-phase flow restricts one phase to a collection of particles dispersed in the other phase, the continuous carrier fluid. The particles interact with the carrier fluid by modulation of turbulence and by exchange of momentum, mass and energy. Depending on the volume fraction of the dispersed phase and the size of the particles, different interaction mechanisms have to be accounted for. The classification of two-phase flow on the basis of these interactions is presented in section 3.1.

The turbulent one-phase flow description presented in the previous chapter, can be classified as a model, due to the acceptance of the Boussinesq assumption, the k-ε models, the modelling of the molecular momentum transport with Newton’s Law of Viscosity and the molecular thermal energy transport with Fourier’s Law of Heat Conduction.

The turbulent particulate two-phase flow description is not yet in that stadium. The work done on the two-phase problem has resulted into two approaches. One approach is called Euler-Lagrange, the other Euler-Euler. The Eulerian approach to the description of a phase is presented in chapter 2. The flow is taken as a continuum and the field is resolved on a fixed, three-dimensional grid. The values on the grid nodes represent the local averages of the continuous flow field. The Lagrangian approach to the description of a phase is to represent the phase by particles, where the history of the particle position, velocity and optionally other varying properties, such as temperature, diameter, density and component mass fractions are calculated based on the particle motion equations presented in section 3.2. Averaging these values around discrete positions in time and place, results in a flow field, which is the equivalent of the Eulerian flow field. The two approaches to the two-phase flow problem are presented in section 3.3. In that section derivations will be presented, from which the different formulations of two-phase flow in the literature can be analyzed. Because of the assumptions needed for the derivation, this analysis is restricted to non-rotating particles only.

The present state of the art is presented in the section on turbulence modulation, where the two approaches come together to formulate the terms needed to describe
Table 3.1: Coupling of dispersed two-phase flows as a function of particle volume fraction $\alpha_p$

<table>
<thead>
<tr>
<th>Coupling Type</th>
<th>$\alpha_p$ Domain</th>
<th>Coupling Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>One-way coupling</td>
<td>$\alpha_p &lt; 10^{-6}$</td>
<td>Particle-motion is effected by the fluid motion: Turbulent dispersion.</td>
</tr>
<tr>
<td>Two-way coupling</td>
<td>$10^{-6} &lt; \alpha_p &lt; 10^{-3}$</td>
<td>Turbulence modulation by particles. Turbulent dispersion of particles.</td>
</tr>
<tr>
<td>Four-way coupling</td>
<td>$\alpha_p &gt; 10^{-3}$</td>
<td>Next to the two-way coupling the particle-particle interaction is taken into account using collision models.</td>
</tr>
</tbody>
</table>

the effect of the presence of particles on turbulence.

3.1 Coupling in Two-Phase Flow

Dispersed two-phase flow is classified by Sommerfeld [9] with regard to the importance of interaction mechanisms (Table 3.1) into very dilute, dilute and dense flows. For very dilute flows (dispersed phase volume fraction $\alpha_p < 10^{-6}$) only the effect of the fluid motion on the particles is taken into account. This is called one-way coupling.

The dilute flow is characterized by two-way coupling. Here the particle presence effects the turbulence, which in turn disperses the particles.

For dense dispersed two-phase flows ($\alpha_p > 10^{-3}$) the particle-particle interaction becomes important. Collisions models must be used and the average particle distance becomes a characteristic length for the turbulent flow, in addition to the Kolmogorov length-scale. Kenning and Crowe [22] propose a new hybrid length scale $l_h = (1/L_e + 1/\lambda)^{-1}$, composed of the integral length scale $L_e$ and the average particle distance $\lambda$ as a characterization of particulate multi-phase flow. $L_e$ is empirically determined to be one tenth of a pipe diameter and $\lambda \approx d_p[(\pi/6\alpha_d)^{1/3} - 1]$, where $d_p$ is the particle diameter and $\alpha_d$ is the dispersed phase volume fraction. The modulation predicted on the basis of this length scale agrees with experimental data, implying that the use of point particles, to simulate turbulence in fluid-particle systems will not capture the contribution due to inter-particle spacing. See also section 3.4. The coupling between particles and between particles and turbulent flow is called the four-way coupling problem and should not be considered completely solved.

3.2 Particle Motion Equations

Because the formulation of the Eulerian dispersed phase equations rely on the particle motion equations, these have to be presented first.
In Lagrangian analysis the particles, which form the dispersed phase, are usually not tracked individually, but are assumed to travel along the same trajectory with a number of other particles, in order to reduce the computational power needed. The trajectory is calculated for a particle, which represents the whole group: a parcel of particles. These parcels are treated as point-like, in the sense that their size and shape enter into the computation only via the semi-empirical drag coefficient.

The tracking is done by solving the particle motion equation and the thermal energy equation. These equations, which account for the change in position, velocity and thermal energy, provide together with the parcel initial conditions a closed system for the modelling of trajectories. A trajectory is the collection of different positions in the fluid a parcel occupies before leaving the calculation domain. The equations for a particle with mass $m_p$ for respectively position, velocity and thermal energy are:

$$
\frac{dx_{i,p}}{dt} = v_{i,p} \\
\frac{mv_{i,p}}{dt} = \sum F_{i,r} \\
m_p \frac{d(c_{p,p}T_p)}{dt} = -A_{S,p}h(T_p - T_f)
$$

$F_{i,r}$ represents the components of the different relevant forces acting on a particle. $A_{S,p}$ is the particle surface area, $c_{p,p}$ is the particle heat capacity, $h$ is the heat transfer coefficient, $T_p$ is the temperature of the particle and $T_f$ is the local temperature of the fluid. The subscripts $p$ and $f$ refer respectively to the particle and the fluid phase. The heat coefficient is calculated using the Nusselt number:

$$
h = \frac{k_c Nu}{d_p} \quad (3.4)
$$

$$
Nu = 2(1 + 0.3 Re_p^{1/2} Pr^{2/3}) \quad (3.5)
$$

$$
Re_p = \frac{\rho_f d_p |\bar{u}_f - \bar{v}_p|}{\mu_f} \quad (3.6)
$$

Where $k_c$ is the thermal conductivity of the continuous phase, $Nu$ is the Nusselt number, $d_p$ is the particle diameter, $Re_p$ is the particle Reynolds number, $Pr$ is the Prandtl number and $\mu_f$ is the fluid phase molecular viscosity.

### 3.2.1 Eddy life time model

To model the effect of turbulent dispersion on the particles the eddy life time model has been developed. (See also the section 3.3.2 on Eulerian Dispersed Phase Equations, especially equation 3.75.) In the eddy life time model turbulent flow is regarded as a collection of turbulent eddies with discrete velocities and life times. The fluid velocity encountered by the particle is constant during the time the particle remains in an eddy. The fluid velocity $u_{i,f}$ is taken as the sum of the local time averaged fluid velocity $\bar{u}_{i,f}$ and a fluctuating velocity $u'_{i,f}$ selected from a Gaussian distribution with a variance proportional to the turbulence kinetic energy ($\sigma^2 = \frac{2k}{3}$).
The length scale of the turbulent eddy is estimated to be

\[ l_{edd} = C_\mu k \frac{3}{\epsilon} \] (3.7)

and the eddy life time \( T_E \) as

\[ T_E = \frac{l_{edd}}{\sqrt{\frac{2k}{3}}} \] (3.8)

where \( \epsilon \) is the dissipation rate and \( C_\mu \) is an empirical constant (see table 2.1). The residence time of a particle in an eddy due to a relative velocity between the particle and the eddy is:

\[ T_R = \frac{l_{edd}}{|u - v|} \] (3.9)

The interaction time between the fluid and the turbulent eddy can now be defined as the minimum of the eddy life time and the residence time:

\[ T_I = \min(T_R, T_E) \] (3.10)

The particle is assumed to be in the eddy for the duration of the interaction time and then in a new eddy. Using the eddy life time model the Lagrangian time step size is identical to \( T_I \) or does not sample new fluctuating velocities in time steps smaller than \( T_I \) for the duration of \( T_I \). The fluid velocities in the definitions of the particle forces are the velocities generated by the eddy life time model.

### 3.2.2 Particle forces

**Drag force:**

\[ F_{D,i} = \frac{3}{4} \frac{m_p}{d_p^2} \frac{\rho_f}{\rho_p} C_D (u_i - u_i^p) (|\vec{u}_f^i - \vec{v}_p|) \] (3.11)

\[ C_D = \begin{cases} 
\frac{24}{Re_p} & \text{for } Re_p \leq 10^3 \\
0.44 & \text{for } Re_p > 10^3 
\end{cases} \] (3.12)

Where \( \rho_f \) and \( \rho_p \) represent the densities and \( d_p \) represents the particle diameter.

**Pressure force and gravity force:**

\[ F_{p,i} = -\frac{m_p}{\rho_p} \frac{\partial \rho}{\partial x_i} \] (3.14)

\[ F_{g,i} = \frac{m_p}{\rho_p} \Delta \rho g_i \] (3.15)

Where \( \Delta \rho \) is the density difference between the carrier and the dispersed phase. Sommerfeld [9] and Lahn [11] combine the force due to the pressure gradient and the shear stress gradient. From the Navier-Stokes equation 2.13 of the fluid the pressure
3.2. PARTICLE MOTION EQUATIONS

gradient and the shear stress can be related to the fluid acceleration and the gravity force:

\[
F_{p,i} = \frac{m_p}{\rho_p} \left( -\frac{\partial p}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} \right) = m_p \frac{\rho_f}{\rho_p} \left( \frac{Du_{i,f}}{Dt} - g_i \right)
\]  

(3.16)

\( \frac{D}{Dt} \) is the material derivative: \( \frac{\partial}{\partial t} + u_{f,i} \frac{\partial}{\partial x_i} \). The gravity force is hereby expressed as

\[
F_{g,i} = m_p g_i
\]  

(3.17)

Transverse lift force as given by Sommerfeld \[12\]:

\[
F_{tl} = \frac{\rho_f \pi d_p^2}{4} C_{tl} d_p \epsilon_{ijk} \epsilon_{klm} (u_{f,j} - u_{p,j}) \frac{\partial u_{f,l}}{\partial x_m}
\]  

(3.18)

Where \( \epsilon_{ijk} \) is the Levi-Civita pseudo-tensor:

\[
\epsilon_{ijk} = \begin{cases} 
1 & \text{when } ijk \text{ is an even permutation of } 123 \\
-1 & \text{when } ijk \text{ is an odd permutation of } 123 \\
0 & \text{when any two indexes have the same value}
\end{cases}
\]

And \( C_{tl} \) is the lift coefficient:

\[
C_{tl} = \frac{4.1126}{Re_S^{0.5}} f(Re_p, Re_S)
\]  

(3.19)

The correlation function \( f(Re_p, Re_S) \) for a particle Reynolds number in the range \( 0.1 \leq Re_p \leq 100 \) is given by:

\[
f(Re_p, Re_S) = (1 - 0.3314 \beta^{1/2}) e^{-\frac{Re_p}{10}} + 0.3314 \beta^{1/2} \quad \text{for: } Re_p \leq 40
\]

\[
0.0524 (\beta Re_p)^{1/2} \quad \text{for: } Re_p \geq 40
\]

(3.20)

With:

\[
\beta = 0.5 \frac{Re_S}{Re_p}
\]  

(3.21)

And the Reynolds number of the rotational flow:

\[
Re_S = \frac{\rho_f d_p^2 |\nabla \times \vec{u}_f|}{\mu_f}
\]  

(3.22)

Where \( |\nabla \times \vec{u}_f| \) is the magnitude of the rotation of the flow. Particles moving in a shear layer experience a transverse lift force due to the non-uniform relative velocity over the particle and the resulting non-uniform pressure distribution. The lift force is acting toward the direction of the higher slip velocity. When the particle Reynolds number \( Re_p \) is very small the transverse lift force is also known as the Saffman force and \( f(Re_p, Re_S) = 1 \).
CHAPTER 3. PARTICULATE TWO-PHASE FLOW

**Added mass force.** The added mass or virtual mass force is the force required to accelerate the carrier fluid entrained by the droplet:

\[
\overrightarrow{F}_{am} = -0.5 \rho_f \frac{d\overrightarrow{a}_f}{dt} 
\]  

(3.23)

The forces taken into account differ from case to case (Table 3.2). Sommerfeld states (page 18 of [9]) that in liquid solid flows the pressure force is important since \(\rho_f/\rho_p \approx 1\).

<table>
<thead>
<tr>
<th>Simulated case</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air bubbles in a water column</td>
</tr>
<tr>
<td>Stationary turbulent spray</td>
</tr>
<tr>
<td>Numerical study into Eulerian and Lagrangian predictions of particulate two-phase flow.</td>
</tr>
<tr>
<td>Gas-liquid flow</td>
</tr>
<tr>
<td>Particles in air. Up to 2% of volume</td>
</tr>
<tr>
<td>Particle laden slab flow</td>
</tr>
</tbody>
</table>

**Table 3.2: Forces taken into account**

<table>
<thead>
<tr>
<th></th>
<th>(F_D)</th>
<th>(F_p)</th>
<th>(F_{am})</th>
<th>(F_{tl})</th>
<th>(F_g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lain</td>
<td>[11]</td>
<td>(F_D)</td>
<td>(F_p)</td>
<td>(F_{am})</td>
<td>(F_{tl})</td>
</tr>
<tr>
<td>Sommerfeld</td>
<td>[19]</td>
<td>(F_D)</td>
<td>(F_p)</td>
<td>(F_{am})</td>
<td>(F_{tl})</td>
</tr>
<tr>
<td>Durst</td>
<td>[6]</td>
<td>(F_D)</td>
<td>(F_p)</td>
<td>(F_{am})</td>
<td>(F_{tl})</td>
</tr>
<tr>
<td>Sokolichin</td>
<td>[13]</td>
<td>(F_D)</td>
<td>(F_p)</td>
<td>(F_{am})</td>
<td>(F_{tl})</td>
</tr>
<tr>
<td>Stojanovic</td>
<td>[14]</td>
<td>(F_D)</td>
<td>(F_p)</td>
<td>(F_{am})</td>
<td>(F_{tl})</td>
</tr>
<tr>
<td>Vermorel</td>
<td>[17]</td>
<td>(F_D)</td>
<td>(F_p)</td>
<td>(F_{am})</td>
<td>(F_{tl})</td>
</tr>
</tbody>
</table>

### 3.3 Euler/Euler vs. Euler/Lagrange approach

In this section the different formulations of two-phase flow are derived, preceded by a short introduction into the basis characterizations of two-phase flow. The derivation of the formulation presents the results together with the assumptions, so that deviating formulations in literature can be assessed as wrong or as having different assumptions, most importantly the dependence between the positioning of the volume fraction \(\alpha\) and the formulation of the momentum source term. Two-phase flow is characterized by volume or mass averaged properties. In contrast to one-phase flow the minimum volume over which is averaged is not determined by the number of molecules, but by the number of particles. So while the mono-phase, material density \(\rho_c\) can be defined as

\[
\rho_c \equiv \lim_{\delta V \to 0} \frac{\delta M}{\delta V},
\]

(3.24)

the continuous phase bulk density is defined as

\[
\overline{\rho}_c \equiv \lim_{\delta V \to V_c} \frac{\delta M_c}{\delta V}.
\]

(3.25)
3.3. **EULER/EULER VS. EULER/LAGRANGE APPROACH**

Where \( M_c \) is the mass of the continuous phase and \( V_o \) is the limiting volume that ensures a stationary average. This means that \( V_o \) is dependent on the (local) composition of the two-phase flow. A more formal criterion for volume averaging is given with the definition of the local volume average (3.34) and the phase average (3.33). Other properties of two-phase flow can be defined in the same way:

\[
n \equiv \lim_{\delta V \rightarrow V_o} \frac{\delta N}{\delta V} \tag{3.26}
\]

\[
\alpha_c \equiv \lim_{\delta V \rightarrow V_o} \frac{\delta V_c}{\delta V} \tag{3.27}
\]

Giving a different definition for the bulk density:

\[
\bar{\rho}_c = \alpha_c \rho_c \tag{3.28}
\]

Where \( n \) is the particle number density and \( \alpha_c \) is the continuous phase volume fraction. Changing the subscripts \( c \) to \( d \), gives the dispersed phase properties. Using these definitions the mixture properties can be defined as:

\[
\rho_m \equiv \bar{\rho}_c + \bar{\rho}_d = \alpha_c \rho_c + \alpha_d \rho_d \tag{3.29}
\]

\[
C \equiv \frac{\bar{\rho}_d}{\bar{\rho}_c} \tag{3.30}
\]

\[
z \equiv \frac{m_d}{m_c} = \frac{\bar{\rho}_d V}{\bar{\rho}_c u} \tag{3.31}
\]

\[
Z \equiv \frac{M_d}{M_c} \tag{3.32}
\]

Where \( \rho_m \) is the mixture density, \( C \) is the mass concentration, \( z \) is the loading and \( Z \) is the total loading.

In the following subsections the equations for the Eulerian approach to the continuous phase, the equations for the Eulerian approach to the dispersed phase and the equations for the Lagrangian approach are presented. However, in this section only the continuity, the momentum and the thermal energy equations will be presented. In the next section on turbulence modulation the \( k-\epsilon \) equations will be presented for both Euler-Euler and Euler-Lagrange approach.

### 3.3.1 The Eulerian Continuous Phase Equations

The continuous phase equations are derived by taking the volume average of the continuity (2.8), the Navier-Stokes (2.12) and the incompressible thermal-energy (2.16) equations of section 2.2, while taking into account the presence of a volume fraction \( \alpha_d \) of the dispersed phase. This leads to volume averaged equations, which include the source terms representing the interaction between the phases. Therefore the formulas for averaging are introduced first, after which the aforementioned equations will be averaged.

The derivation shows the dependence between the formulation of the source terms and the position of the continuous phase volume fraction within the transport equations.
Local Volume and Phase average

The phase average is the average over the volume of the continuous phase and is defined as:

$$\langle B \rangle \equiv \frac{1}{V_c} \int_{V_c} B dV$$  \hspace{1cm} (3.33)

Where $B$ is some property of the continuous phase per unit volume.

The local volume average is defined as:

$$\bar{B} \equiv \frac{1}{V} \int_{V_c} B dV = \frac{V_c}{V} \frac{1}{V_c} \int_{V_c} B dV = \alpha_c(B)$$  \hspace{1cm} (3.34)

Where $V = V_c + V_d$ is the control volume, over which the averaging is performed.

A more general statement regarding the minimum size of the averaging volume $V_o$ is now possible. If the averaging volume is displaced over a distance corresponding to the linear dimension of the volume ($V^{1/3}$), then the phase average properties should not change. This implies that

$$\langle \bar{B} \rangle = \bar{B}$$  \hspace{1cm} (3.35)

If this implication is fulfilled then the equations which are derived by averaging the partial differentials of section 2.2, can still be considered point equations with respect to the volume averaged properties.

When there is no volume change of the dispersed phase with time, such as evaporation or condensation, the volume average of the time derivative is:

$$\bar{\frac{\partial B}{\partial t}} = \frac{\partial \bar{B}}{\partial t}$$  \hspace{1cm} (3.36)

The volume average of a gradient operation introduces an extra term, due to the presence of the dispersed phase:

$$\bar{\frac{\partial B}{\partial x_i}} = \frac{\partial \bar{B}}{\partial x_i} - \frac{1}{V} \int_{S_d} B n_i dS$$  \hspace{1cm} (3.37)

Where $S_d$ is the total dispersed phase surface area in the averaging volume, and $n_i$ is the unit normal vector directed outward from the dispersed phase. The new term on the right-hand-side accounts for the effects of the volume integral over $V_c$ on non-uniformities of $B$ on surface $S_d$. When they arise in the coming derivations a physical explanation is given. A formal derivation of these averages can be found in appendix B of Crowe, Sommerfeld and Tsuji [7], which gives the basis for the derivations.

Averaging the Continuity equation

Volume averaging 2.8 gives:

$$\frac{\partial p_c}{\partial t} + \frac{\partial p_c u_i}{\partial x_i} - \frac{1}{V} \int_{S_d} p_c u_i n_i dS = 0$$  \hspace{1cm} (3.38)
3.3. EULER/EULER VS. EULER/LAGRANGE APPROACH

Defining the mass averaged velocity $\bar{u}_i$ as:

$$\bar{u}_i \equiv \frac{1}{\langle \rho_c \rangle} \frac{1}{V_c} \int_{V_c} \rho_c u_i dV$$

(3.39)

then with $u_i = \bar{u}_i + \delta u_i$, the volume averaged transport term becomes:

$$\bar{\rho_c} \bar{u}_i = \frac{1}{V_c} \int_{V_c} \rho_c u_i dV = \alpha_c \bar{u}_i(\rho_c)$$

(3.40)

In the surface integral over the dispersed phase surface $S_d$, $\rho_c$ is replaced with $\rho_{cs}$, which is the average continuous phase density at the particle-surface, and $u_i$ is replaced with $v_i$, which is the velocity of the particle center, implying no change in distance from surface to center with time and no rotation. Because neither $\rho_{cs}$ nor $v_i$ depend on the surface integral, this results in

$$\frac{1}{V} \int_{S_d} \rho_{cs} u_i n_i dS = \frac{1}{V} \rho_{cs} v_i \int_{S_d} n_i dS = 0$$

(3.41)

Collecting the terms and substituting them in 3.38, gives the continuous phase continuity equation:

$$\frac{\partial}{\partial t} (\alpha_c(\rho_c)) + \frac{\partial}{\partial x_i} (\alpha_c(\rho_c) \bar{u}_i) = 0$$

(3.42)

Averaging the Navier-Stokes Equation

Volume averaging 2.12 gives:

$$\frac{\partial (\rho_c u_i)}{\partial t} = - \frac{\partial}{\partial x_j} (\rho_c u_j u_i) - \frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial p}{\partial x_i} + \rho_c g_i$$

(3.43)

The time derivative becomes:

$$\frac{\partial (\rho_c u_i)}{\partial t} = \frac{\partial \rho_c u_i}{\partial t} = \frac{\partial}{\partial t} (\alpha_c \bar{u}_i(\rho_c))$$

(3.44)

The transport term becomes:

$$\frac{\partial}{\partial x_j} (\rho_c u_j u_i) = \frac{\partial}{\partial x_j} \rho_c (\bar{u}_j + \delta u_j)(\bar{u}_i + \delta u_i) - \frac{1}{V} \int_{S_d} \rho_c u_j u_i n_i dS$$

(3.45)

Again replacing $u_i$ with $v_i$ and $u_j$ with $v_j$ in the surface integral, makes the integral term zero, because the product $v_i v_j$ is constant with respect to the integral. Rearranging results in:

$$\frac{\partial}{\partial x_j} (\rho_c u_j u_i) = \frac{\partial}{\partial x_j} (\alpha_c(\rho_c) \bar{u}_j \bar{u}_i + \alpha_c(\rho_c \delta u_j \delta u_i))$$

(3.46)

The second term is the stress due to fluctuations, which is equivalent to the Reynolds stress in single phase flow. Important difference is that the flow does not have to be

$^1$This means no condensation or evaporation.
turbulent to create this stress, since fluctuations can be caused by the flow around the particles.

Introducing \( p = \langle p \rangle + \delta p \) the volume average of the pressure gradient becomes:

\[
\frac{\partial p}{\partial x_i} = \frac{\partial \langle p \rangle}{\partial x_i} - \frac{1}{V} \int_{S_d} p n_i \, dS = \frac{\partial}{\partial x_i} (\alpha_c(p)) - \frac{1}{V} \int_{S_d} (\langle p \rangle + \delta p) n_i \, dS
\]

The second term on the right-hand-side represents the contribution to the pressure gradient in the continuous phase equation due to the presence of particles and the pressure-force on the particles by the continuous phase. The control volume surface \( S \) slides for a fraction \( \alpha_d \) through particles, defining \( S_s = \alpha_d S \). The slid particles form a blocked surface \( S_b \) for the continuous phase convective transport through \( S \). The dispersed phase surface \( S_d \) is composed of \( S_b \) and the particle surface \( S_i \) of particles entirely inside the averaging volume. A surface integral over \( S_c \) as well as one over \( S_s \) and \( S_b \), thus over closed volumes, is zero.\(^2\) Therefore a surface integral over \( S_s \) has the same magnitude as one over \( S_b \). Thus the integral terms become:

\[
\frac{1}{V} \int_{S_s} \langle p \rangle n_i \, dS + \frac{1}{V} \int_{S_s} \langle p \rangle n_i \, dS = -\frac{1}{V} \int_{S_s} \langle p \rangle n_i \, dS + 0 =
\]

\[
= -\frac{1}{V} \int_S \alpha_d \langle p \rangle n_i \, dS = -\frac{\partial}{\partial x_i} (\alpha_d(p))
\]

The negative sign appears because \( n_i \) is directed inward into the control volume at \( S_b \) and outward of the control volume at \( S_s \). While \( \langle p \rangle \) is dependent on the averaging volume surface \( S \) integral, it is constant with respect to the \( S_i \) integral. Therefore the pressure term becomes:

\[
\frac{\partial p}{\partial x_i} = \frac{\partial}{\partial x_i} (\alpha_c(p)) + \frac{\partial}{\partial x_i} (\alpha_d(p)) - \frac{1}{V} \int_{S_d} \delta p n_i \, dS =
\]

\[
= \frac{\partial (\langle p \rangle + \delta p)}{\partial x_i} - \frac{1}{V} \int_{S_d} \delta p n_i \, dS
\]

Where the second term on the right hand side is the pressure force on the particles. Introducing \( \tau_{ij} = \langle \tau_{ij} \rangle + \delta \tau_{ij} \) and following the same procedure with the volume average of the gradient of the shear stress gives:

\[
\frac{\partial \tau_{ij}}{\partial x_j} = \frac{\partial \langle \tau_{ij} \rangle}{\partial x_j} - \frac{1}{V} \int_{S_d} \delta \tau_{ij} n_j \, dS
\]

Where the second term on the right hand side is the force due to viscous stress on the particles inside the averaging volume. The integral of the pressure force and the viscous stress on all the interior surfaces \( S_d \) is equal to the hydrodynamic forces (lift and drag) on the particles in the volume. Thus:

\[
\frac{1}{V} \int_{S_d} (-\delta p n_i - \delta \tau_{ij} n_j) \, dS = \frac{1}{V} \sum_k F_{i,k}
\]
3.3. EULER/EULER VS. EULER/LAGRANGE APPROACH

Where \( F_{i,k} \) represents the \( i^{th} \)-component of the hydrodynamic force on particle \( k \). The hydrodynamic force on a particle can be rewritten to explicitly include the pressure gradient and the shear stress gradient. From section 3.2 the hydrodynamic forces on a particle \( k \) can be expressed as:

\[
\frac{1}{V} \sum_k F_{i,k} = \sum_k (-V_{d,k} \frac{\partial(p)}{\partial x_i} - V_{d,k} \frac{\partial(\tau_{ij})}{\partial x_j} + L_{i,k}) = -\alpha_d \frac{\partial(p)}{\partial x_i} - \alpha_d \frac{\partial(\tau_{ij})}{\partial x_j} + \frac{1}{V} \sum_k L_{i,k}
\]  

(3.52)

Where \( V_d \) is the particle volume and \( L_i \) is the rest of the surface forces acting on the particle, namely lift force, steady-state drag force, and virtual mass force. Collecting the terms and substituting them in 3.43, gives the continuous phase momentum equation:

\[
\frac{\partial}{\partial t}(\alpha_c \vec{u}_i(\rho_c)) = -\frac{\partial}{\partial x_j}(\alpha_c(\rho_c)\vec{u}_j \vec{u}_i) - \alpha_c \frac{\partial(p)}{\partial x_i} + \alpha_c \frac{\partial(\tau_{ij})}{\partial x_j} + \frac{\partial(u_i \tau_{ij})}{\partial x_j} + \alpha_c \rho_c g_i - \frac{1}{V} \sum_k L_{i,k}
\]  

(3.53)

Worth noting is that the \( \alpha_c \) appearing on the right hand side of the equation before the gradient terms of pressure and shear stress is different in origin from the \( \alpha_c \) in the gravity term.

Averaging the thermal energy equation

Volume averaging 2.16 gives:

\[
\frac{\partial (\rho_c c_p T_c)}{\partial t} = -\frac{\partial (\rho_c u_i c_p T_c)}{\partial x_i} = \frac{\partial q_i}{\partial x_i} + \frac{\partial (u_i \tau_{ij})}{\partial x_j}
\]  

(3.54)

Defining the mass averaged thermal energy \( \overline{c_p T_c} = \langle \rho_c c_p T_c \rangle/\langle \rho_c \rangle \), the time derivative becomes:

\[
\frac{\partial (\overline{\rho_c c_p T_c})}{\partial t} = \frac{\partial \rho_c \overline{c_p T_c}}{\partial t} = \frac{\partial (\alpha_c(\rho_c) \overline{c_p T_c})}{\partial t}
\]  

(3.55)

With \( c_p T_c = \overline{c_p T_c} + \delta(c_p T_c) \), the transport term becomes:

\[
\frac{\partial (\rho_c u_i(c_p T_c))}{\partial x_i} = \frac{\partial \rho_c (\vec{u}_i + \delta \vec{u}_i)(c_p \overline{T_c} + \delta(c_p T_c))}{\partial x_i} - \frac{1}{V} \int_{S_d} \rho_c c_p T_c u_i n_i dS = \frac{\partial}{\partial x_i} (\alpha_c(\rho_c) \overline{c_p T_c} \overline{u}_i + \alpha_c(\rho_c \delta u_i \delta(c_p T_c)) + \frac{1}{V} \rho_c c_p T_c v_i \int_{S_d} n_i dS = \frac{\partial}{\partial x_i} (\alpha_c(\rho_c) \overline{c_p T_c}) + \frac{\partial}{\partial x_i} \alpha_c(\rho_c \delta u_i \delta(c_p T_c)) - 0
\]  

(3.56)
CHAPTER 3. PARTICULATE TWO-PHASE FLOW

In the surface integral over $S_d$, $\rho_c$ is replaced by $\rho_{cs}$, which is the average density of the continuous phase at the surface $S_d$, $T_c$ by the temperature of the particle surface $T_p$ and $u_i$ by the velocity $u_i$ of the particle mass center. These replacements are constant with respect to the surface integral, making the latter zero. The average of the gradient in the heat flux becomes:

$$\frac{\partial q_i}{\partial x_i} = \frac{\partial \overline{q_i}}{\partial x_i} - \frac{1}{V} \int_{S_d} q_{i,n}dS$$  \hspace{1cm} (3.57)

The second term on the right-hand-side represents the heat flow to the particles and the contribution of the particles to the heat flow through the continuous phase. The heat transfer around a droplet can be expressed as the sum of an average value over the surface and a deviation therefrom,

$$q_i = \overline{q_i} + \delta q_i$$  \hspace{1cm} (3.58)

As explained in the text before equation 3.48, $S_d$ is composed of $S_e$ and $S_b$, giving:

$$\frac{1}{V} \int_{S_e} q_{i,n}dS = \frac{1}{V} \int_{S_e} \overline{q_{i,n}}dS$$  \hspace{1cm} (3.59)

$$\frac{1}{V} \int_{S_b} q_{i,n}dS = \frac{1}{V} \int_{S_b} \overline{q_{i,n}}dS - \frac{1}{V} \int_{S_e} \delta q_{i,n}dS$$  \hspace{1cm} (3.60)

The last term represents the heat transfer to the continuous phase through the droplets, which are sliced by the averaging volume surface. The surface integral over $S_d$ containing $\overline{q_i}$ is the net heat transfer to the continuous phase from the droplets and can be rewritten as:

$$\frac{1}{V} \int_{S_e+S_b} \overline{q_i,n}dS = \frac{1}{V} \sum_k \hat{Q}_k$$  \hspace{1cm} (3.61)

Where $\hat{Q}_k$ is the net heat transfer from droplet $k$ to the fluid.

This results in:

$$\bar{\frac{\partial q_i}{\partial x_i}} = \frac{\partial q_{i,eff}}{\partial x_i} - \frac{1}{V} \sum_k \hat{Q}_k$$  \hspace{1cm} (3.62)

Where $q_{i,eff} = \alpha_c(q_i) + \alpha_d(\delta q_i)$ or $q_{i,eff} = -k_{eff}(T_c)/\partial x_i$, where $k_{eff}$ is the effective thermal conductivity for the mixture.

The averaged gradient of the work rate due to shear stress becomes:

$$\overline{\frac{\partial (u_i \tau_{ij})}{\partial x_j}} = \frac{\partial \overline{u_i \tau_{ij}}}{\partial x_j} - \frac{1}{V} \int_{S_d} u_i \tau_{ij}n_j dS$$  \hspace{1cm} (3.63)

Assuming Newton’s Law of viscosity: $\tau_{ij} = -\mu \frac{\partial u_i}{\partial x_j}$ this can be rearranged into:

$$\frac{\partial}{\partial x_j}(-\mu \frac{\partial (\frac{1}{2}u_i^2)}{\partial x_j}) - \frac{1}{V} \int_{S_d} -\mu \frac{\partial (\frac{1}{2}u_j^2)}{\partial x_j} n_j dS$$  \hspace{1cm} (3.64)
Replacing in the integral over \( S_d \) \( u_i \) with \( v_i \), which is the velocity of the mass center of a particle, where \( v_i^2 \) and \( \frac{\partial (\frac{1}{2} v_i^2)}{\partial x_j} \) are constant with respect to the integration over \( S_d \), gives:

\[
\frac{\partial (u_i v_{ij})}{\partial x_j} = - \frac{\partial}{\partial x_j} \left( \frac{\partial (\frac{1}{2} \mu (u_i + \delta u_i)^2)}{\partial x_j} \right) = \\
- \frac{\partial}{\partial x_j} \left( \mu \frac{\partial (\alpha_c \frac{1}{2} \tilde{u}_i^2)}{\partial x_j} + \alpha_c \frac{1}{2} \tilde{u}_i \delta (\frac{1}{2} \tilde{u}_i^2) \right) = \\
- \frac{\partial}{\partial x_j} \left( \mu \frac{\partial (\alpha_c \frac{1}{2} \tilde{u}_i^2)}{\partial x_j} \right) - \frac{\partial}{\partial x_j} \left( \mu \frac{\partial (\alpha_c \frac{1}{2} \tilde{u}_i^2)}{\partial x_j} \right)
\]

(3.65)

These two assumptions (no-slip condition on non-rotating particle surface and Newtonian fluid behavior) together imply that the power due to viscous stress on the particles can be neglected. The more general neglect of viscous stress on particles would reduce the pressure force (3.16) to the pressure-term (3.14) only, thereby not changing the momentum equation for the continuous phase.

Collecting the terms and substituting them in 3.54, gives the continuous phase volume averaged thermal energy equation:

\[
\frac{\partial}{\partial t} \left( \alpha_c \langle \rho_c \rangle c_p T_c \right) = - \frac{\partial}{\partial x_i} \left( \alpha_c \langle \rho_c \rangle \tilde{u}_i c_p T_c \right) + \frac{\partial q_{i, eff}}{\partial x_i} + \\
- \frac{\partial}{\partial x_i} \left( \alpha_c \langle \rho_c \delta u_i \delta (c_p T_c) \rangle \right) - \frac{\partial}{\partial x_j} \left( \mu \frac{\partial (\alpha_c \frac{1}{2} \tilde{u}_i^2)}{\partial x_j} \right) + \\
- \frac{\partial}{\partial x_j} \left( \mu \frac{\partial (\alpha_c \frac{1}{2} \tilde{u}_i^2)}{\partial x_j} \right) - \frac{1}{V} \sum_k \dot{Q}_k
\]

(3.66)

In appendix B of the book on Multi-phase Flow ([7]) a more general approach to the derivation of the thermal energy equation is worked out, which is also valid for compressible flow.

### 3.3.2 Two-Fluid Model - The Dispersed Phase Equations

The two-fluid model is an Euler/Euler approach to two-phase flow. It consists of the continuous phase equations derived in the previous subsection together with the dispersed phase equations, which are presented in this subsection. First some basic definitions are introduced, which couple particle size class properties to dispersed phase properties, after which the continuity, the momentum and the thermal energy equations are presented.

**Basic definitions**

The volume averaged velocity of the dispersed phase is defined as:

\[
\langle v \rangle = \frac{\sum_k v_k}{N}
\]

(3.67)
Where \( v_k \) is a characteristic velocity of a particle in size-class \( k \) and \( N \) is the number of particles within the averaging volume.

The Favre or mass averaged velocity is defined as:

\[
\bar{v} = \frac{\sum_k m_k v_k}{\sum_k m_k}
\]  
\[ (3.68) \]

Where \( m_k \) is the mass of a particle in size-class \( k \).

The mass flow-rate \( \dot{M} \) through a surface \( A \) is:

\[
\dot{M} = \sum_k n_k m_k v_k A = \rho_d \bar{v} A
\]  
\[ (3.69) \]

Where \( \rho_d \) is the dispersed phase bulk density \( \bar{v} \) is identified in terms of particle size class properties as \( \sum_k n_k m_k \), in which \( n_k \) is the number density of particles in size-class \( k \).

**Dispersed phase continuity equation**

Over a box of volume \( V_o \) as implied by equation 3.35 the mass balance of the dispersed phase particles is:

\[
\frac{\Delta (V_o \rho_d)}{\Delta t} = \sum_{i=1}^{3} \left( \rho_d \bar{v}_i A \bigg|_{x_i} - \rho_d \bar{v}_i A \bigg|_{x_i + \Delta x_i} \right)
\]  
\[ (3.70) \]

Where \( \Delta x_i A = V_o \). Dividing by \( V_o \) gives the mass averaged dispersed phase continuity equation:

\[
\frac{\partial (\alpha_d \rho_d)}{\partial t} = -\frac{\partial (\alpha_d \rho_d \bar{v}_i)}{\partial x_i}
\]  
\[ (3.71) \]

If the simple average velocity is used, in lieu of the mass averaged velocity, the continuity equation has to be formulated differently. In this case the velocity, the bulk density and consequently the mass flux in the averaging volume are expressed as:

\[
v_i = \langle v_i \rangle + \delta v_i
\]  
\[ (3.72) \]

\[
\rho_d = \rho_{d,0} + \delta \rho_d
\]  
\[ (3.73) \]

\[
\langle \rho_d v_i \rangle = \langle \rho_d \rangle \langle v_i \rangle + \langle \delta \rho_d \delta v_i \rangle
\]  
\[ (3.74) \]

Where \( \delta \rho_d \) is the deviation in bulk density in adjacent averaging volumes. The additional term can be regarded as a mass diffusion term. In a flow with homogeneous bulk density or uniform particle velocities this term would be zero. Turbulence, however will produce a distribution of particle velocities which will give rise to a net mass flux in non-homogeneous particle density fields.
3.3. EULER/EULER VS. EULER/LAGRANGE APPROACH

The gradient transport model is used in the two-fluid formulation to simulate dispersion of particles in turbulent flow. With reference to Fick's law it is assumed that

\[ (\delta p_d \delta v_i) = -D_d \frac{\partial p_d}{\partial x_i} \]  

(3.75)

where \( D_d \) is the dispersion coefficient for the dispersed phase. The value for the dispersion coefficient has to be determined from fitting with experimental data. A further problem exists with the boundary conditions for bulk density. The gradient of bulk density can be assumed to be zero at a wall if particles bounce specular, but not if the particles do not bounce mirror-like.

The final form of for the two-fluid continuity equation using the volume averaged velocity is:

\[ \frac{\partial}{\partial t} (\alpha_d p_d) = -\frac{\partial}{\partial x_i} (\alpha_d p_d (v_i)) + \frac{\partial}{\partial x_i} \left( D_d \frac{\partial p_d}{\partial x_i} \right) \]  

(3.76)

**Dispersed phase momentum equation**

To derive the momentum equation, the material derivative of the dispersed phase momentum over the averaging volume \( V_o \) is equated to the sum of the Lagrangian changes of momentum for each size class \( k \), within the volume \( V_o \):

\[ \frac{D(V_o \delta p_d \delta v_i)}{Dt} = \sum_k \frac{\partial(m_k v_{i,k})}{\partial t} \]  

(3.77)

where

\[ \frac{D(V_o \delta p_d \delta v_i)}{Dt} = \frac{1}{V_o} \left( \frac{\partial (\delta p_d \delta v_i)}{\partial t} + \frac{\partial}{\partial x_j} \left( \sum_k n_k m_k v_{j,k} v_{i,k} \right) \right) \]  

(3.78)

and

\[ \sum_k \frac{\partial(m_k v_{i,k})}{\partial t} = \sum_k \left( - V_k \frac{\partial}{\partial x_i} - V_k \frac{\partial}{\partial x_j} (\sum_i \alpha_d \frac{\partial(p)}{\partial x_i} + \sum_i \frac{\partial(\tau_{ij})}{\partial x_j} \right) \]

\[ + L_{i,k} + V_k \rho_d k g_i \]  

(3.79)

Where \( V_k \) is the characteristic size of a particle in size class \( k \), and \( L_{i,k} \) is the fluid force on a particle of size class \( k \) excluding the forces due to the pressure and shear stress gradients.

Let \( v_{i,k} = \tilde{v}_{i,k} + \delta v_{i,k} \). Dividing equation 3.77 by \( V_o \), substituting the terms and rearranging, gives:

\[ \frac{\partial(\alpha_d p_d \tilde{v}_i)}{\partial t} = -\frac{\partial}{\partial x_i} (\alpha_d p_d \tilde{v}_j \tilde{v}_i) - \alpha_d \frac{\partial(p)}{\partial x_i} - \alpha_d \frac{\partial(\tau_{ij})}{\partial x_j} + \]

\[ + \alpha_d p_d g_i + \frac{1}{V} \sum_k L_{i,k} - \frac{\partial}{\partial x_j} \left( \sum_k \rho_{d,k} \delta v_{j,k} \delta v_{i,k} \right) \]  

(3.80)

Where the particle class \( k \) bulk density \( \overline{p}_{d,k} = m_k n_k \). The last term is the dispersed phase Reynolds stress:

\[ \tau_{d,ij} = - \sum_k \overline{p}_{d,k} \delta v_{k,j} \delta v_{k,i} \]  

(3.81)
The dispersed phase Reynolds stress arises because the mass averaged velocity is not a momentum averaged velocity. Usually it is modelled with the Boussinesq approximation (stress proportional to the rate of strain):

\[ - \sum_k \bar{p}_{d,k} \delta v_{i,k} \delta v_{j,k} = \mu_s \left( \frac{\partial \bar{v}_i}{\partial x_i} + \frac{\partial \bar{v}_j}{\partial x_j} \right) - \frac{2}{3} \mu_s \frac{\partial \bar{v}_k}{\partial x_k} \delta_{ij} \]  

(3.82)

Where \( \mu_s \) is the solids viscosity. It is very difficult to select a solids viscosity since the particle velocity fluctuations depend not only on local turbulence but also on the particle properties and history. A work-around is to simply use a constant ratio between the solids viscosity and the fluid eddy viscosity. The problem with the Boussinesq approximation is that the dispersed phase Reynolds stress can be non-zero without the presence of strain, due to turbulent fluctuations of particle velocities.

Again problems arise with the boundary conditions for the velocity. The velocity tangential to a wall does not need to be zero for particles. For dilute flows the information is transmitted along particle trajectories and is thus parabolic in nature, whereas a fluid is elliptic, because information is transmitted in all directions by pressure waves. Setting up boundary conditions for the dispersed phase for the two-fluid model for dilute flow is always problematic.

In the traditional two-fluid model for a dense phase flow, the force on the particles due to shear stress in the continuous phase is neglected and another term is added to account for the particle-particle interaction. The differential form of the momentum equation for non-evaporating dense phase flow is [7]:

\[ \frac{\partial}{\partial t} \left( \alpha_d \rho_d \bar{v}_i \right) = - \frac{\partial}{\partial x_j} \left( \alpha_d \rho_d \bar{v}_j \bar{v}_i \right) - \frac{\partial \tau_{d,ij}}{\partial x_j} - \alpha_d \frac{\partial p}{\partial x_i} - G \frac{\partial \alpha_d}{\partial x_i} + \beta_V (u_i - \bar{v}_i) + \alpha_d \rho_d g_i \]  

(3.83)

Where \( G \) is the solids stress modulus obtained from empirical formulas and the term \( \beta_V (u_i - \bar{v}_i) \) represents the fluid force on the dispersed phase, excluding the pressure force. This term will be defined in equation 3.85. This model has been used to predict flow properties, including cluster formation, in circulating fluidized beds [8].

**Dispersed phase thermal energy equations**

In full analogy with the momentum equation derivation, the thermal energy equation for the dispersed phase becomes:

\[ \frac{\partial}{\partial t} \left( \alpha_d \rho_d c_p \bar{T}_d \right) = - \frac{\partial}{\partial x_i} \left( \alpha_d \rho_d \bar{v}_i c_p \bar{T}_d \right) + \frac{1}{V} \sum_k \dot{Q}_k + \]  

\[ - \frac{\partial}{\partial x_i} \left( \sum_k \bar{p}_{d,k} \delta v_{i,k} \delta (c_p T_{d,k}) \right) \]  

(3.84)

Where \( D_{d,k} \) is the characteristic diameter of size class \( k \). The last term is analogous to the Reynolds stress and has to be modelled with a gradient diffusion term. If the variations in droplet temperature are small this term can be neglected.
3.3. EULER/EULER VS. EULER/LAGRANGE APPROACH

Coupling terms in the two-fluid model

The basic problem of the two-fluid model is to redefine the interaction terms into source term with no reference to the sum of particle properties. Crowe [24] expressed the fluid-dynamic force acting on the fluid per unit volume of mixture as:

\[
\frac{1}{V} \sum_k L_{i,k} = n 3 \pi \mu_c d_p f(\ddot{v}_i - \ddot{u}_i) = \beta_V(\ddot{v}_i - \ddot{u}_i) \tag{3.85}
\]

Where \( \mu_c \) is the viscosity of the carrier phase, \( d_p \) is the particle diameter, \( f \) is the ratio of the drag coefficient to the Stokes drag and \( \beta_V \) is a constant, introduced for easy writing. Assumed is that the particle size is uniform and \( f \) is constant. Other forces than the drag force are not considered.

In [7] Crowe expresses the heat transfer from the particles to the fluid in the averaging volume as:

\[
\dot{Q}_d = N N u \pi k_c d_p cp \dot{T}_d - \dot{T}_c \tag{3.86}
\]

Where \( N \) is the number of particle in the averaging volume, \( Nu \) is the Nusselt number around a particle (see equation 3.5, \( k_c \) is the conductivity of the continuous phase and \( d_p \) is the uniform particle diameter. The source term in the thermal energy equation becomes:

\[
\frac{1}{V} \sum_k \dot{Q}_k = n N u \pi k_c d_p (cp \dot{T}_d - cp \dot{T}_c) = \beta_T(cp \dot{T}_d - cp \dot{T}_c) \tag{3.87}
\]

Where \( n \) is the number density and \( \beta_T \) is a constant, introduced for easy writing.

The problem with the introduction of these source terms for the two-fluid model is the transformation of a two-fluid problem in a multi-fluid problem if the particles cannot be characterized by one uniform diameter. In Euler-Euler modelling a separate set of dispersed phase equations has to be solved for every size class.

Summary of two-fluid model

\[
\frac{\partial}{\partial t}(\alpha_c(\rho_c)) = - \frac{\partial}{\partial x_i}(\alpha_c(\rho_c)\ddot{u}_i) \tag{3.88}
\]

\[
\frac{\partial}{\partial t}(\alpha_d(\rho_d)) = - \frac{\partial}{\partial x_i}(\alpha_d(\rho_d)\ddot{u}_i) \tag{3.89}
\]

\[
\frac{\partial}{\partial t}(\alpha_c\ddot{u}_i(\rho_c)) = - \frac{\partial}{\partial x_j}(\alpha_c(\rho_c)\ddot{u}_j\ddot{u}_i) - \alpha_c \frac{\partial (p)}{\partial x_i} - \alpha_c \frac{\partial (\tau_{ij})}{\partial x_j} + 
\]

\[
\frac{\partial}{\partial x_j}(\alpha_c(\rho_c)\ddot{u}_j\ddot{u}_i) + \alpha_c \rho_c g_i + \beta_V(\ddot{u}_i - \ddot{u}_i) \tag{3.90}
\]

\[
\frac{\partial}{\partial t}(\alpha_d(\rho_d)\ddot{u}_i) = - \frac{\partial}{\partial x_j}(\alpha_d(\rho_d)\ddot{u}_j\ddot{u}_i) - \alpha_d \frac{\partial (p)}{\partial x_i} - \alpha_d \frac{\partial (\tau_{ij})}{\partial x_j} + 
\]

\[
\frac{\partial}{\partial x_j}(\alpha_d(\rho_d)\ddot{u}_j\ddot{u}_i) + \alpha_d \rho_d g_i + \beta_V(\ddot{u}_i - \ddot{u}_i) \tag{3.91}
\]
3.3.3 Euler-Lagrange analysis

The Euler-Lagrange analysis consists of the tracking of particles through a Eulerian continuous phase. The particle-motion can be simulated with the equations derived in the section on particle equations. From these trajectories interaction terms with the continuous phase can be calculated. These source terms change the continuous phase fields, which in turn change the trajectories and the calculated source terms. Iterations are needed before the Eulerian flow-field is converged.

The weak points of the Euler-Euler approach, which are dilute flow (non-elliptic information transmittance) and multi-size classed particle distributions (multiple sets of dispersed phase equations), are the strong points of Lagrangian analysis. Most publications on Euler-Lagrangian analysis are about very low particle volume fraction, so that the continuous phase equations reduce to:

\[
\frac{\partial}{\partial t} \langle \rho_c \rangle = -\frac{\partial}{\partial x_i} \langle \rho_c \rangle \tilde{u}_i
\]

\[
\frac{\partial}{\partial t} \langle \tilde{u}_i \rho_c \rangle = -\frac{\partial}{\partial x_j} \langle \rho_c \rangle \tilde{u}_i \tilde{u}_j - \frac{\partial \rho_c}{\partial x_j} \tilde{u}_j - \frac{\partial \langle \tau_{ij} \rangle}{\partial x_j} + \frac{\partial \langle p \rangle}{\partial x_j} \tilde{u}_j + \rho_c g_i - \frac{1}{V} \sum_k L_{i,k} \tag{3.98}
\]

\[
\frac{\partial}{\partial t} \langle \rho_c \tilde{c}_p T_c \rangle = -\frac{\partial}{\partial x_i} \langle \rho_c \rangle \tilde{c}_p \tilde{T}_c + \frac{\partial q_{i,\text{eff}}}{\partial x_i} + \frac{\partial \langle \tau_{ij} \rangle}{\partial x_j} \tilde{u}_j - \frac{\partial \rho_c \delta u_i \delta (c_p T_c)}{\partial x_j} - \mu \frac{\partial^2 \tilde{u}_j}{\partial x_j^2} + \frac{\partial \langle \tau_{ij} \rangle}{\partial x_j} \tilde{u}_j + \frac{1}{V} \sum_k \tilde{Q}_k \tag{3.99}
\]

When Newton’s Law of Viscosity, Fourier’s Law of Heat Conduction and the Boussinesq approximation are introduced, these equations are identical to the single phase
3.4 TURBULENCE MODULATION

Equations presented in chapter 2, summarized in section 2.7 with the exception of the interaction terms and the dependence of the molecular viscosity \( \mu \) on temperature and thereby on space-coordinates. Defining these interaction terms as the source terms \( S_{\phi d} \), the general form of the equations of the continuous phase becomes:

\[
\frac{\partial ((\rho_c)\phi)}{\partial t} = -\frac{\partial (\bar{u}_j \rho \phi)}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \Gamma_{\phi} \frac{\partial \phi}{\partial x_j} \right) + S_\phi + S_{\phi d}
\] (3.100)

Where \((\rho)\) is the volume averaged continuous phase density, \( \bar{u}_j \) is the mass averaged velocity component, \( \Gamma_{\phi} \) is an effective gradient transport term for the scalar \( \phi \), \( S_\phi \) is the source term for \( \phi \) and \( S_{\phi d} \) is the interaction term.

The change in momentum of a particle is due fluid hydrodynamic force \( L_{i,k} \), the pressure force and the gravity. Therefore the source term \( \langle S_{u_{i,d}} \rangle \) for the momentum equation is:

\[
-\frac{1}{V} \sum_k L_{i,k} = \langle S_{u_{i,d}} \rangle = n\left(-\left(m_p \frac{dp_{p,i}}{dt} - F_{p,i} - m_p g_i\right)\right)
\] (3.101)

The source term for the thermal energy \( \langle S_{c_p T_{d,d}} \rangle \) is the sum over the change of thermal energy of all particles in the averaging volume:

\[
-\frac{1}{V} \sum_k \dot{Q}_k = \langle S_{c_p T_{d,d}} \rangle = n\left(-m_p \frac{dc_p T_p}{dt}\right)
\] (3.102)

With these extra source terms and the other values for the continuity, momentum and thermal energy equations as presented in table 2.2, the only problem remaining are the \( k \) and \( \epsilon \) equations. This problem emerges from the fact that the presence of particles modulates the turbulence. The turbulence can be attenuated or augmented. Because of this source terms have to be introduced into the k-\( \epsilon \)-model equations.

3.4 Turbulence Modulation

The presence of particles can affect the carrier phase turbulence in several ways such as:

- displacement of the flow field by flow around a dispersed phase element,
- generation of wakes behind particles,
- dissipation of turbulence due to transfer of turbulence energy to the motion of the dispersed phase,
- modification of velocity gradients in the carrier flow field and corresponding change in turbulence generation,
- introduction of additional length scales which may effect the turbulence dissipation,
- disturbance of flow due to particle-particle interaction.
Two criteria are suggested for suppression and enhancement of turbulence. One criterion is based on the length scale ratio $d_p/L_ε$, where $d_p$ is the particle diameter and $L_ε$ is the length scale characteristic of the eddies with the most energy. In pipes $L_ε \approx 0.1D$, where $D$ is the pipe diameter. It is observed that turbulence intensity is attenuated for $d_p/L_ε$ less than 0.1 while the turbulence level is increased for larger length scale ratios. Presented by Gore and Crowe [21] this criterion assumes that the turbulent length scale of the carrier phase does not change with the addition of particles. But this could be due to the narrow range of particle diameters for which data is present. Empirically the strongest evidence is for gas-solid pipes and jets. The other criterion is based on the relative particle Reynolds number $. This criterion suggests that particles with high particle Reynolds number tend to increase turbulence and particles with low particle Reynolds number tend to suppress the fluid turbulence. According to Stojanovic [14], (who refers to Yarin and Hetzroni (1994)), turbulence production due to the presence of particles should be expected at values of particle Reynolds number greater than 110. Kenning and Crowe [22] write that Hetzroni’s (1989) critical particle Reynolds number, which is based on dimensional analysis, is 400. In Crowe, Sommerfeld and Tsuji’s basic work [7] the first criterion is preferred.

Calculation methods for turbulence modulation are still in development. The general approach is to modify the generation and dissipation terms in the $k$-$ε$ equations to account for the presence of the dispersed phase. In the next subsections the standard terms, the Crowe terms and the consistent terms will be introduced. These three groups of terms give an account of the history of the development and the status of the various terms.

### 3.4.1 Standard Terms in $k$-$ε$ Equations

Treating the properties of the continuous phase momentum equation (3.98) in the Euler-Lagrange approach as values at a point, the procedure is to first multiply equation (3.98) by the velocity to obtain a mechanical energy equation, express the velocities as an average value plus a deviation, take a temporal average and subtract the average mechanical energy equation to yield an equation for the turbulence kinetic energy. Hereby following the same procedure as outlined in chapter 2, formulated in equation 2.34. So the only change to the $k$-equation as presented in chapter 2 is the introduction of the source term $S_{k,d}$ due to interaction with the dispersed phase, which is the transformed source term $S_{ui,d}$ of the momentum equation:

$$
S_{k,d} = \frac{\delta u_i \delta S_{ui,d}}{u_i S_{ui,d} - \bar{u}_i S_{ui,d}} = \frac{(\bar{u}_i + \delta u_i)(S_{ui,id} + \delta S_{ui,d}) - \bar{u}_i S_{ui,d}}{u_i S_{ui,d} - \bar{u}_i S_{ui,d}}
$$

(3.103)

This formulation of $S_{k,d}$ is referred to as the standard term. The term $S_{ui,d}$ represents the instantaneous contact force that the particle exerts on the fluid.

The modelling of the analogous term in the $ε$-equation is performed in the standard manner, which assumes that the additional production or destruction of dissipation is proportional to $S_{k,d}$ and is the inverse of the turbulent characteristic time-scale $C_L k/ε$ (Gouesbet [18]). Grouping the coefficient $C_L$ with the proportionality con-
3.4. TURBULENCE MODULATION

It is possible to write:

\[ S_{\epsilon,d} = C_3 \frac{e}{\epsilon} S_{k,d} \]  

(3.104)

The adequacy of \( S_{\epsilon,d} \) is controversial, particularly in combination with the standard term for \( S_{k,d} \). It is an ad hoc parameterization of the effect of particles on the dissipation rate and the value for the constant \( C_3 \) is not universal, but depends most likely on volume fraction and particle density.

Crowe ([24] and [23]) has argued against the standard term. His first argument is that \( S_{\epsilon,d} \) includes the drag force per unit volume of mixture and cannot be regarded as a force at a point in the flow. The momentum equation that applies to a point is the Navier-Stokes equation (2.13) which does not include a momentum coupling term.

His second point is that in a packed bed with steady and uniform flow (no temporal or spatial gradients in the averaged properties) one would expect that the turbulence generated by the fixed particles would be dissipated by viscous forces. Using Crowe’s two-fluid formulation of the momentum coupling term (3.85) the k-equation becomes:

\[
\frac{\partial k}{\partial t} = -\rho_c \bar{u}_i \frac{\partial k}{\partial x_i} + \frac{\partial}{\partial x_j} \left( \Gamma \frac{\partial k}{\partial x_j} \right) - \rho_c \bar{u}_i \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} - \beta \nu \left( \bar{u}_i \bar{u}_i - \delta \bar{u}_i \bar{u}_i \right) - \rho_c \epsilon
\]  

(3.105)

Where the continuous phase density \( \rho_c \) is assumed constant and the turbulent dissipation is resolved according to equation (2.38) with DNS. Applying the above equation to the packed bed flow configuration; that is, setting \( \partial/\partial t \) and \( \partial/\partial x_i \) equal to zero, gives

\[-\beta \nu \bar{u}_i \bar{u}_i - \rho_c \epsilon = 0 \]  

(3.106)

which is incorrect since the dissipation \( \epsilon \) is always positive. Crowe concludes by stating that the problem lies in taking averaged values as being local values and treating the equations as if they represent a single phase flow with a local coupling term. In the next subsection Crowe’s coupling terms will be presented.

3.4.2 Crowe’s Terms

Crowe’s approach [23] in deriving the turbulence energy equation for a fluid-particle mixture is to use the mechanical energy equation for the fluid phase of an incompressible fluid, namely,

\[
\rho_c \frac{D}{Dt} \left( \frac{u_i u_i}{2} \right) = -\frac{\partial}{\partial x_i} (u_i p) - u_j \frac{\partial}{\partial x_j} \tau_{ij} + \rho_c u_i g_i
\]  

(3.107)

The velocities, pressure and shear stress are expressed as the sum of the volume-averaged quantities and the deviation form these values,

\[
u_i = \langle u_i \rangle + \delta u_i, p = \langle p \rangle + \delta p, \tau_{ij} = \langle \tau_{ij} \rangle + \delta \tau_{ij}
\]  

(3.108)
These values are substituted in the mechanical energy equation and the resulting equation is volume averaged. The product of the volume averaged velocity and the momentum equations (3.92) is subtracted to yield an equation for the turbulence kinetic energy. The resulting equation is

\[
\frac{\partial}{\partial t}(\alpha_c \rho_c k_c) =
\]

- transport of \( k_c \)

\[
- \frac{\partial}{\partial x_i} \left( \alpha_c \rho_c \langle u_j \rangle k_c \right)
\]

- diffusion of \( k_c \)

\[
+ \frac{\partial}{\partial x_j} \left( \Gamma \frac{\partial k_c}{\partial x_j} \right)
\]

- generation by gradients

\[
- \alpha_c \rho_c \langle \delta u_i \delta u_j \rangle \frac{\partial \langle u_i \rangle}{\partial x_j}
\]

- generation by particle drag

\[
+ \beta_V \left( \langle u_i \rangle - \langle v_i \rangle \right)^2
\]

- redistribution

\[
+ \beta_V \left( \langle \delta u_i \delta v_i \rangle - \langle \delta u_i \delta v_i \rangle \right)
\]

- dissipation

One identifies two terms associated with the presence of the dispersed phase. One terms reflects the conversion of mechanical work by the drag force into turbulence kinetic energy and the other, the redistribution term, represents the transfer of kinetic energy of the particle motion to kinetic energy in the carrier fluid. This term represents four-way coupling. In dilute flow it is usually small compared to the particle drag generation term but it becomes important in dense phase flows when particle-particle collisions are a sink of particle kinetic energy.

### 3.4.3 Laín’s Consistent Terms

Although Crowe’s terms together with the proportional coupling term in the \( \epsilon \)-equation would suffice for a Euler-Lagrange analysis, the main drawback is the lack of consideration for other forces than the drag-force, the pressure force and gravity effects. (Remember that for the derivation of the momentum coupling term it was expressed as the hydrodynamic force acting on the particles excluding the pressure force. See subscript at equation 3.79.) While for Crowe’s solid/gas systems this might be feasible, the bubbly motion in the flow studied by Laín [11] is described taking the added or virtual mass force and the transverse lift force into consideration. Although Laín doesn’t exclude the possibility of a derivation including all these forces, he has a different solution. The supposedly local interaction force \( S_{u_i,d} \) takes place at the surface of a particle, therefore, if particle rotation and evaporation are excluded, the fluid velocity is equal to the particle velocity. This allows him to formulate his consistent term:

\[
S_{k,d} = \frac{\nu_i S_{u_i,d} - \bar{u}_i S_{u_i,d}}{v_i}
\]  

(3.110)

If only the drag force is considered in \( S_{u_i,d} \) with the assumption of mono-dispersed spherical particle (see equation 3.85) equation 3.110 reduces to the Crowe terms:

\[
S_{k,d} = \frac{\nu_i \beta_V \langle u_i - u_i \rangle - \bar{u}_i \beta_V \langle u_i - u_i \rangle}{\beta_V \left( \left( \bar{u}_i + \delta u_i \right) \left( \bar{u}_i + \delta u_i \right) - \left( \bar{u}_i + \delta u_i \right) \left( \bar{u}_i + \delta u_i \right) \right)}
\]
3.5 FINAL FORM OF THE MODEL EQUATIONS FOR TWO-PHASE FLOW

\[ \beta_v \left( \overline{u_i^2} + \overline{\delta u_i^2} - 2\overline{u_i u_i} + \overline{\delta v_i \delta u_i - \delta u_i \delta v_i} \right) = \beta_v \left( \overline{u_i - \overline{u}_i} \right)^2 + \beta_v \left( \overline{\delta v_i \delta u_i - \delta u_i \delta v_i} \right) \]  \hspace{1cm} (3.111)

Lain's arguments for his terms are

- the aforementioned inclusion of additional forces,
- the fact that the Crowe terms consider the particles mostly as a source of dissipation, as only the last part of the term may give a negative contribution to \( S_{k,d} \), and
- the experimental validation or tuning of the constants appearing in the proportional \( S_{\epsilon,d} \) term.

He thereby heads Crowe's theoretical experiment of the packed bed, ignoring at the same time the fact that the drag force is a volume averaged term, appearing in a volume averaged equation.

Lain states that his formulation of \( S_{k,d} \) is only a first approximation as long as rotation and deformation of the dispersed elements are not considered. Within the research group around Sommerfeld his formulation has success even in a publication on dense three-phase flow, in which rotation is taken in account [20].

3.5 Final form of the model equations for two-phase flow

To simulate dense two-phase turbulent flow with constant material densities the model equations should take into account the dispersed phase fraction. The continuity equation 3.42, the momentum equation 3.53, the thermal energy equation 3.66 and the turbulent energy equation 3.109 are presented, but the turbulent dissipation equation is absent, since Crowe resolved \( \epsilon \) according to 2.38 with DNS.

The only full set of equations for turbulent flow is Lain's set. He sets \( \alpha_c \) equal to 1 and restricts the use of the model to dispersed phase fractions below 2%. He has tuned the constants in his model to dense two-phase flow of air bubbles rising in water. Adapting Lain's model to the Cartesian coordinate system this results to an extension of the table of section 2.7 with the particle source terms \( S_{\phi,d} \) and changes in the model constants and the \( \Gamma_{\phi} \) terms. Lain's model is extended with the thermal energy equation of section 3.3.3. Table 3.3 presents the terms in the general equation for Lagrangian two-phase flow, which has been introduced in equation 3.100.
Table 3.3: The general two-phase equation and the terms for each flow-characteristic.

\[
\frac{\partial (\rho \phi)}{\partial t} = -\frac{\partial (\rho \vec{u}_j \phi)}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \Gamma_\phi \frac{\partial \phi}{\partial x_j} \right) + S_\phi + S_{\phi d}
\]

<table>
<thead>
<tr>
<th>(\phi)</th>
<th>(\Gamma_\phi)</th>
<th>(S_\phi)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(-\frac{\partial (\rho)}{\partial x_i}) + (\rho g_i)</td>
<td>0</td>
</tr>
<tr>
<td>(\vec{u}_i)</td>
<td>(\mu + \mu_t)</td>
<td>(-\frac{\partial (\rho \vec{u}_i \phi)}{\partial x_i})</td>
</tr>
<tr>
<td>(\rho c_p T)</td>
<td>(\frac{\mu_\epsilon}{\epsilon} + \frac{\mu_k}{\epsilon})</td>
<td>(-\frac{\partial}{\partial x_j} \left( \mu \frac{\partial (\frac{1}{2} \vec{u}_j^2 + k)}{\partial x_j} \right))</td>
</tr>
<tr>
<td>(k)</td>
<td>(\frac{\mu k}{\epsilon})</td>
<td>(\rho P - \rho \epsilon)</td>
</tr>
<tr>
<td>(\epsilon)</td>
<td>(\frac{\mu k}{\epsilon})</td>
<td>(C_{\epsilon 1} \frac{\rho \epsilon}{k} P - C_{\epsilon 2} \frac{\rho \epsilon^2}{k})</td>
</tr>
</tbody>
</table>

Where \(P = \nu_i \frac{\partial \phi_i}{\partial x_i} \) and \(\mu_t = C_\mu \frac{k^2}{\epsilon}\)

<table>
<thead>
<tr>
<th>(\phi)</th>
<th>(S_{\phi d})</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>(\vec{u}_i)</td>
<td>(\langle S_{\phi_i, d} \rangle)</td>
</tr>
<tr>
<td>(\rho c_p T)</td>
<td>(\langle S_{\epsilon, d} \rangle)</td>
</tr>
<tr>
<td>(k)</td>
<td>(S_{k, d})</td>
</tr>
<tr>
<td>(\epsilon)</td>
<td>(S_{\epsilon, d})</td>
</tr>
</tbody>
</table>

\(C_\mu = 0.09, C_{\epsilon 1} = 1.44, C_{\epsilon 2} = 1.92, C_{\epsilon 3} = 1.8, \sigma_k = 1, \sigma_\epsilon = 1.3\). Model equations for constant density, non-reactive, two-phase turbulent flow. Where \(\rho\) is the continuous phase density, \(\vec{u}_i\) is a volume averaged velocity component, \(x_j\) is the direction of the velocity component, \(\Gamma_\phi\) is an effective gradient transport term for the scalar \(\phi\), \(S_\phi\) is the source term for \(\phi\) and \(S_{\phi d}\) is the phase-interaction term.
Chapter 4

Numerical Analysis

4.1 Introduction

The equations of change derived in the previous chapters are non-linear partial differential equations (PDE). Given the appropriate boundary conditions and these PDE's, the properties of the flow-field are fixed. Because the PDE's are non-linear and interdependent no analytical solution is possible. Instead of representing the field by its varying properties as functions of time and space-coordinates, the field is represented by a collection of positions at which the values of the characteristic parameters are determined at different instants of time. At these points, the aforementioned nodes of the grid, the values of the properties $\bar{u}_i$, $\langle p \rangle$, $c_p T$, $k$ and $\epsilon$ will be determined.

By setting the values of the boundary nodes and resolving the interdependence of the field values of the parameters, the field is determined. The interdependency relations between the nodal values and their direct neighbors in time and space are algebraic relations derived from the equations of change of the volume averaged properties, which are represented in the general form in tables 2.2 and 3.3. Deriving the algebraic relation between a nodal value and its neighbors from the general form, with subsequent substitution of $\phi$ by its particular counterparts gives the particular algebraic equations.

The derivation entails two steps. First the general equation of change is integrated over a finite volume around the node over a finite time step. (This step is the reverse of the shrinking of a box to a point of section 2.2. Although this seems to be rather a roundabout: starting with a box, shrinking to zero, volume averaging, fluctuation modelling, general equation, integrating back to box; this way did provide us with the means to model turbulent flow with a start for modelling multiphase flow.) And secondly the gradients present need to be approximated by nodal values and geometrical factors.

Given the boundary values and algebraic relations, the field is solved by an iterative algorithm. Two algorithms will be treated. The Semi Implicit Method for Pressure Linked Equations (SIMPLE) algorithm and the Pressure Implicit Splitting of Operators (PISO) algorithm.

For Lagrangian analysis the particle motion equations are discretized, solved and
from the resulting trajectories the particle source terms $S_{psd}$ are calculated. In the last two sections the discretization of the particle equations and the calculation of the particle source terms are treated.

### 4.2 Finite Volume approach

#### Geometrical Definition

Following Patankar's notation [25] the node in the control volume is designated by $P$. In a three dimensional grid $P$ is surrounded in space by six other nodes at its west-, east-, north-, south-, top- and bottom-side, respectively the nodes $W$, $E$, $N$, $S$, $T$ and $B$. See figure 4.1 for a 2D grid representation. The distances between $P$ and its neighbors are respectively $(\delta x)_{w}$, $(\delta x)_{e}$, $(\delta x)_{n}$, $(\delta x)_{s}$, $(\delta x)_{t}$ and $(\delta x)_{b}$. $P$ is taken as being inside a box of six sides, each side being an interface between the control volume of $P$ and the control volume of one of its neighbors. The part of $(\delta x)_{w}$ between $P$ and the interface is $(\delta x)_{w}^{-}$, between $W$ and the interface is $(\delta x)_{w}^{+}$. The position of the other interfaces is defined in the same way, replacing $w$ with respectively $e$, $n$, $s$, $t$ and $b$.

#### Derivation of the algebraic equation

The integrated general form is:

$$
\int_{V} \int_{t}^{t+\Delta t} \frac{\partial}{\partial t} (\rho \phi) dt dV = \int_{t}^{t+\Delta t} \int_{V} \nabla \cdot (\rho \vec{v} \phi) dV dt + \int_{t}^{t+\Delta t} \int_{V} \nabla \cdot \left( \Gamma \frac{\partial \phi}{\partial x} \right) dV dt + \int_{t}^{t+\Delta t} \int_{V} S_{\phi} + S_{psd} dV dt
$$

Where $V$ is the control volume around $P$ and $\Delta t$ the time step over which is integrated.

Assuming the grid-point value $\rho \phi P$ prevails throughout the control volume, then $A$ becomes:

$$
A \approx \rho \phi P V \Big|_{t+\Delta t} - \rho \phi P V \Big|_{t}
$$

When the new value is denoted by the superscript $n$ and the old value by the superscript $o$, this becomes:

$$
A \approx (\rho \phi P V)^{n} - (\rho \phi P V)^{o}
$$
4.2. FINITE VOLUME APPROACH

Using the divergence theorem:

$$\int_V \nabla \vec{B} dV = \int_{S_V} \vec{B} \hat{n} dS$$  \hspace{1cm} (4.4)

Where $\hat{n}$ is a unit vector normal to the surface element $dS$ pointing outward, $\vec{B} \hat{n}$ is the component of $\vec{B}$ in the direction of the vector $\hat{n}$. And given that $S_V$ is the sum of the six sides of the control volume, results in:

$$B = \int_t^{t+\Delta t} \left( \sum_k \Gamma_k \left( \frac{\partial \phi}{\partial x_j} \right)_k \hat{n}_k A_k \right) dt$$  \hspace{1cm} (4.5)

Where $k = w, e, n, s, t, b$ sums over the six sides with surface area $A_k$. Defining $K = W, E, N, S, T, B$, the value of $\Gamma_k$ at interface $k$ becomes:

$$\Gamma_k = \left( \frac{1 - f_k}{\Gamma_P} + \frac{f_k}{\Gamma_K} \right)^{-1}$$  \hspace{1cm} (4.6)

Where $f_k \equiv \frac{(\delta x)_k}{(\delta x)_\infty}$ and $K$ is coupled to $k$.

To calculate gradients at the control volume faces an approximate distribution of properties between the nodal points is used. Linear approximations seem to be the most obvious and simplest way of calculating interface values and gradients. This practice is called central differencing (CD). The last equation (4.5) can then be approximated as:

$$B \approx \int_t^{t+\Delta t} \sum_k \Gamma_k \left( \frac{\phi_K - \phi_P}{(\delta x)_k} \right) A_k dt$$  \hspace{1cm} (4.7)

Approximating the time integral of $\phi$ over $\Delta t$ as:

$$\int_t^{t+\Delta t} \phi_P dt \approx [f \phi_P^0 + (1 - f) \phi_P^0] \Delta t$$  \hspace{1cm} (4.8)

Where $f$ is a weighting factor. When the time integral is evaluated based only on the old nodal value(s), $f = 0$, it is called the explicit scheme. When based only on the new value(s), $f = 1$, it is called the implicit scheme. When $f = 0.5$ in the above equation, it is known as the Crank-Nicholson scheme.

Then the approximation for $B$ becomes:

$$B \approx \left[ f \left( \sum_k \Gamma_k \left( \frac{\phi_K - \phi_P}{(\delta x)_k} \right) A_k \right)^n \right. + (1 - f) \left( \sum_k \Gamma_k \left( \frac{\phi_K - \phi_P}{(\delta x)_k} \right) A_k \right)^0 \] \Delta t$$  \hspace{1cm} (4.9)

Taking the source terms as averages over volume and time, $C$ becomes:

$$C = (\langle S' \phi \rangle + \langle S'_{\phi\phi} \rangle) V \Delta t$$  \hspace{1cm} (4.10)
CHAPTER 4. NUMERICAL ANALYSIS

Where the over-bars represent averaging over time.

D becomes:

\[ D = \int_{t}^{t+\Delta t} \sum_{k} -\rho \vec{u}_k \phi_k \vec{n}_k A_k \]

\[ \approx \left[ f \left( \sum_{k} -\rho \vec{u}_k \phi_k \vec{n}_k A_k \right) \right]^{n} \]

\[ + (1 - f) \left( \sum_{k} -\rho \vec{u}_k \phi_k \vec{n}_k A_k \right)^{o} \Delta t \]

(4.11)

Where \( \vec{u}_k = \vec{u}_k \cdot \vec{e}_k \), where \( \vec{e}_k \) is the unit vector in the k-direction, and \( \vec{u}_k \) and \( \phi_k \) are the interface k values of respectively the Favre averaged velocity and the scalar \( \phi \).

Patankar suggests a staggered grid: the nodes of the velocity are at the interface of the control volumes for the scalar values, so no interpolation for velocity is needed. Interpolation schemes for these values of \( \phi \) from the nodal values are for example the central difference (CD) scheme, the upwind (UD) scheme and the quadratic upstream interpolation for convective kinetics (QUICK) scheme (See table 4.1). The UD scheme assigns the upstream nodal value to the interface value. The CD scheme takes the central difference of the nodal values between which the interface is. The QUICK scheme takes next to these an extra upstream value into account. Which discretization scheme is to be preferred depends on the \( \phi \)-profile assumptions that can be made.

Table 4.1: Interpolation schemes

<table>
<thead>
<tr>
<th>Scheme</th>
<th>( \phi_k )</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD</td>
<td>( \frac{1}{2}(\phi_P + \phi_K) )</td>
</tr>
<tr>
<td>UD</td>
<td>( \phi_K ) if (</td>
</tr>
<tr>
<td>QUICK</td>
<td>( \phi_P + \frac{1}{3}(3\phi_P - 2\phi_K - \phi_{KK}) ) if (</td>
</tr>
<tr>
<td>QUICK</td>
<td>( \phi_P + \frac{1}{3}(3\phi_K - 2\phi_P - \phi_{PP}) ) if (</td>
</tr>
</tbody>
</table>

Where \( F_k \equiv \rho \vec{u}_k \cdot \vec{n}_k \) represents the normal vector to the surface \( S_k \) pointing outward, \( \phi_{KK} \) is the scalar value at the node once removed from P in the direction of K and \( \phi_{PP} \) is the scalar value at the node next to P, opposite from K. The formulation of the QUICK scheme is strictly valid for uniform grids only.

Introducing the Péclet number:

\[ Pe \equiv \frac{\rho \vec{u}}{\Gamma/\delta x} \]

(4.12)

\( Pe \) can be seen as the ratio of the strengths of convection and diffusion. If \( |Pe| \) for a control volume is smaller than 2 the CD scheme is a good discretization, for larger
values of Pe the UD scheme offers a better discretization of exact solution of the one-dimensional convection-diffusion problem, if $\Gamma$ is taken to be constant. Based on experience this result is generalized in literature, so that for a very small nodal distance $\delta x$ the CD scheme is preferable, while for fast flow through coarse grids the UD scheme is preferable.

When the different schemes are derived with a Taylor-expansion, the order of the difference approximations is the truncated term. The UD scheme is a first order, the CD scheme is a second order and the QUICK scheme is a third order accurate scheme. A negative point of the QUICK scheme is that it can oscillate, making convergence hard or resulting in stabilized oscillations, e.g. lower $\phi$-values at a wall surrounded by higher values. For derivation of the schemes from Taylor-expansions see appendix A of [26].

For the derivation of the algebraic relation from the general formula, $D$ will be discretized with the UD scheme. Defining $\max(a, b)$ to denote the greater of $a$ and $b$, $D$ becomes:

$$
D \approx \left\{ f \left( \sum_k [\phi P \max(-|F_{k} n_{k}|, 0)] + 
- \phi_{K} \max(|F_{k} n_{k}|, 0) \right) A_{K} \right\}^{n} + (1 - f) \left( \sum_k [\phi P \max(-|F_{k} n_{k}|, 0)] + 
- \phi_{K} \max(|F_{k} n_{k}|, 0) \right) A_{K}^{n} \Delta t
$$

(4.13)

Gathering all terms and choosing implicit temporal discretization ($f=1$) for simplicity, the algebraic relation between $\phi_{P}^{n}$ and its neighbors in time and space can be expressed as:

$$
\phi_{P}^{n} d_{P}^{n} = \sum_{k} \phi_{K}^{n} d_{K}^{n} + b
$$

(4.14)

where

$$
d_{K}^{n} = A_{k} \left[ \frac{\Gamma_{k}^{n}}{\delta x_{k}} - \max(|F_{k} n_{k}|, 0) \right]
$$

(4.15)

$$
d_{P}^{n} = \sum_{k} (d_{K}^{n} + A_{k} |F_{k} n_{k}|) + \frac{\rho V}{\Delta t}
$$

(4.16)

$$
b = \phi_{P} d_{P} + (\langle \Sigma_{p} \phi \rangle + \langle \Sigma_{p} d \phi \rangle) V
$$

(4.17)

$$
d_{P}^{n} = \frac{\rho V}{\Delta t}
$$

(4.18)

Where $\langle \rangle$ denotes control volume averaging and time averaging.

**Staggered grid for the velocity components**

The use of a staggered grid for the velocity components has two advantages. First no interpolation for the velocity components on the interface has to be performed. Second the presence of the pressure gradient in the source term of the momentum
equations can now be evaluated using the nodal pressure values. In a non-staggered grid the pressure gradient is based on the neighbors nodal pressure values, without accounting the nodal value of the nodal point under consideration. This independence would allow non-physical pressure-fields, such as a checkerboard arrangement with alternating high and low pressures [25][26]. Third the presence of the velocity gradient in the continuity equation can now also be evaluated using the staggered velocity component nodal values.

The six interface positions around P each have six neighbors, which are taken into account when solving the algebraic relations of the velocity components. The shifting of the nodal point under consideration to the staggered nodal points of the velocity components demands a broader designation of the grid nodes. The lines of the grid are indexed so that every node can be designated by three line numbers. The orthogonal lines at which the node is on which the \( \phi_p \)'s are stored, are designated by the capitals F, G and H. The other lines are designated in respect to these. In figure 4.1 a two dimensional under-staggered grid is represented, in which P can be designated by F and G only. The lines on which interfaces of the scalar control volumes are, are designated by f, g and h. Under-staggering refers to the positions of f, g and h in respect to F, G and H. In an understaggered grid these lay between respectively F and F-1, G and G-1 and H and H-1.

Because scalar values are known only for nodes on capitalized indexed lines, scalar values with non-capitalized indices need to be interpolated. For example the value of \( \Gamma_{(f,g,H)} \) is interpolated from \( \Gamma_{(F,G,H)} \) and \( \Gamma_{(F-1,G,H)} \), which are interpolated from respectively \( \Gamma_{(F,G,H)} \) and \( \Gamma_{(F,G-1,H)} \), and \( \Gamma_{(F-1,G,H)} \) and \( \Gamma_{(F-1,G-1,H)} \). Interpolation can be done as described in the previous subsections.

**Momentum equations**

The difficulty in the calculation of the velocity field lies in the unknown pressure field. If the pressure field is known the velocity field can be calculated with algebraic relation presented in equation (4.14). Otherwise the x-momentum equation for the velocity nodal position on the west interface can be expressed as:

\[
(u_1)^n_{(f,G,H)} q^n_{f,G,H} = \sum (u_1)^n_{(nb)} q^n_{(nb)} + (p_{(f,G,H)} - p_{(f-1,G,H)})^n A_{(f,G,H)} + b_{(f,G,H)}
\]

(4.19)

In the new numbering system the neighboring positions, denoted by nb, are \((f-1,G,H)\), \((f+1,G,H)\), \((f,G+1,H)\), \((f,G-1,H)\), \((f,G,H+1)\) and \((f,G,H-1)\). The pressure gradient forms a part of the source term, but is not included in the b-term for the velocity component relations. The d-terms need interpolation from the scalar nodal values, but are essentially the same as in equations 4.15-4.16. For i=2,3 and the other five velocity nodes similar expressions can be derived.
Figure 4.1: 2-Dimensional under-staggered grid indexing by designating a point as the crossing of two indexed lines. Also shown are the standard designations P, S, E, N, W for the nodal points and s, e, n, w for the interface points for the nodal position F,G.
4.3 Semi Implicit Method for Pressure Linked Equations: SIMPLE

The algorithm is essentially a guess-and-correct procedure for the calculation of pressure on the staggered grid arrangement introduced in the previous section. To initiate the SIMPLE calculation process a pressure field \( p^* \) is guessed. Using the velocity components relation (4.19) the velocity fields \( u_i^* \) are solved. Defining the difference between the continuity satisfying \( p \) and \( u_i \) fields and the starred fields as respectively the pressure correction \( p' \) and the velocity component correction \( u_i' \), the relation between the corrections \( p' \) and \( u_i' \) is:

\[
(u_i')^{n}_{(f,G,H)}d_{(f,G,H)}^{n} = \sum (u_i')^{n}_{(nb)}d_{(nb)}^{n} + (p'_i(F,G,H) - p'_i(F-1,G,H))A_{(f,G,H)}
\]

(4.20)

For \( i=2,3 \) similar relations can be derived. At this point the SIMPLE algorithm drops the term \( \sum (u_i')^{n}_{(nb)}d_{(nb)}^{n} \) from the equation, which is remembered in the name: Semi-Implicit. This results in the velocity correction equations for \( u_1 \):

\[
(u_1)_{(f,G,H)} = (u_1)^*_{(f,G,H)} + (p'_i(F,G,H) - p'_i(F-1,G,H))A_{(f,G,H)}
\]

(4.21)

The superscript \( n \) is dropped because all terms are evaluated as the new values. For \( i=2,3 \) similar relations can be derived.

Integrating the continuity equation of the control volume of the node \( P \), that is the position \((F,G,H)\), and replacing the \( u_i \) at the interfaces by the velocity correction equations, results in the pressure correction equation:

\[
n_Pp' = \sum n_Kp'_K + b'
\]

(4.22)

Where

\[
A_K^2 = \rho \cdot d_k
\]

(4.23)

\[
n_P = \sum n_K
\]

(4.24)

\[
b' = \rho [(u_1)^* A_w - (u_1^* A)_e + (u_2^* A)_s +
- (u_2^* A)_n + (u_3^* A)_b - (u_3^* A)_d]
\]

(4.25)

Where \( d_k \) is to be interpolated at all the interfaces. Return to basic subscripting is possible, because the \( p \)-field is stored at the scalar nodes, not on the staggered velocity component grid.

4.3.1 Sequence of Operations

The important operations, in the SIMPLE algorithm, in the order of execution, are:

1. Guess the pressure field \( p^* \).
2. Iteratively solve the velocity component relations to obtain the \( u_i^* \)-fields.
3. Iteratively solve the pressure correction equation to obtain the \( p' \)-field.

4. Calculate \( p \)-field.

5. Calculate \( u \)-fields using the velocity correction equations.

6. Solve the discretization equations of other \( \phi \)'s if they effect the flow field through fluid properties or source terms.

7. Treat the corrected pressure field \( p \) as the new guessed pressure field \( p^* \), return to step 2 and repeat the whole procedure until a converged solution is obtained.

The advantage of SIMPLE is the low number of calculations involved per iteration. The disadvantage is that the pressure correction is good for correcting the velocity field, but does rather a poor job at correcting the pressure field. Therefore many iterations are needed before convergence is reached. Patankar [25] already revised his SIMPLE algorithm: SIMPLER. In this algorithm a velocity field is guessed, from this the pressure field is calculated. Than \( u^* \)- and the \( p' \)-fields are calculated, but only the velocity is corrected with \( p' \), the pressure stays uncorrected, so that it based on a continuity satisfying velocity field. Although SIMPLER has more calculations per iteration, it generally converges faster than SIMPLE. The difference between these algorithms is only in the means and the way to achieve convergence, not on the final solution!

### 4.4 Pressure Implicit Splitting of Operators: PISO

The PISO algorithm is a pressure-velocity calculation procedure developed originally for the non-iterative computation of unsteady compressible flows. PISO involves one predictor step and two corrector steps and may be seen as an extension of SIMPLE, with a further corrector step to enhance it. The equations presented are an adaptation of Versteeg [26].

The predictor stage is characterized by \( p^* \) and \( u^*_1 \), the first corrector stage by \( p^{**} \) and \( u^{**}_1 \), and the second corrector stage by \( p^{***} \) and \( u^{***}_1 \). The first pressure corrector \( p' \) in PISO is defined as:

\[
p^{**} = p^* + p'
\]  

(4.26)

The pressure corrector equation is identical to equation (4.22) of the SIMPLE algorithm. While the \( u^*_1 \) field is calculated by equation (4.19), the corrected velocity fields are based on the neighboring velocity components of the previous stage:

\[
(u_1)^{(f,G,H)}^{***}_1 = \sum \left( u_1^{(f)} (\text{nb})^d_{(nb)} + (p_{(F,G,H)} - p_{(F-1,G,H)})^{***} A_{(f,G,H)} + b_{(f,G,H)} \right)
\]  

(4.27)

\[
(u_1)^{(f,G,H)}^{****}_1 = \sum \left( u_1^{(f)} (\text{nb})^d_{(nb)} + (p_{(F,G,H)} - p_{(F-1,G,H)})^{****} A_{(f,G,H)} + b_{(f,G,H)} \right)
\]  

(4.28)
Similar relations can be derived for $i=2,3$. Defining the second pressure corrector $p''$ as:

$$ p'' = p^{***} - p^{**} $$  \hspace{1cm} (4.29)

Following the same derivation as for the first pressure correction equation the second pressure correction equation becomes:

$$ m_{PP''} = \sum_k m_K p''_K + b'' $$  \hspace{1cm} (4.30)

Where

$$ m_K = \frac{A_k^2}{d_k} $$  \hspace{1cm} (4.31)

$$ m_p = \sum_k m_K $$  \hspace{1cm} (4.32)

$$ b'' = \rho \left[ \left( \frac{A \sum_{nb} (u_{1,nb}^* - u_{1,nb}^s)}{d} \right)_w - \left( \frac{A \sum_{nb} (u_{1,nb}^* - u_{1,nb}^s)}{d} \right)_e \right. $$

$$ + \left( \frac{A \sum_{nb} (u_{2,nb}^* - u_{2,nb}^s)}{d} \right)_s - \left( \frac{A \sum_{nb} (u_{2,nb}^* - u_{2,nb}^s)}{d} \right)_n $$

$$ + \left( \frac{A \sum_{nb} (u_{3,nb}^* - u_{3,nb}^s)}{d} \right)_b - \left( \frac{A \sum_{nb} (u_{3,nb}^* - u_{3,nb}^s)}{d} \right)_t \right] $$  \hspace{1cm} (4.33)

Versteeg writes that for steady flow problems PISO has a more robust convergence for problems in which momentum is not strongly coupled to the scalar variables, than SIMPLER, but SIMPLER for strongly coupled flow problems. Looking from the viewpoint of computational power needed, the Star-CD manual finds SIMPLE too expensive compared to PISO, due to its reliance on an additional level of iteration to handle coupling between variables.

### 4.5 Discretization of Particle Equations

All formulations in this section are taken from the Star-CD manual [10]. The particle equations 3.1-3.3 are discretized into first order Euler-implicit form, respectively:

$$ \frac{x_{i,p}^n - x_{i,p}^p}{\delta t_L} = \dot{v}_{i,p}^n $$  \hspace{1cm} (4.34)

$$ \frac{v_{i,p}^n - u_{i,p}^p}{\delta t_L} = F_{D,i}^n (C_D^o) + F_{p,i}^n + F_{b,i}^n $$  \hspace{1cm} (4.35)

$$ m_p \frac{c_p(T_{p}^n - T_{f}^p)}{\delta t_L} = -A_{S,p} h(T_{p}^n - T_f^p) $$  \hspace{1cm} (4.36)

Where the subscript $p$ signifies the parcel characteristics, the subscript $f$ signifies the carrier fluid characteristics, $C_D^o$ is the drag coefficient based on the old slip
4.6. CALCULATION OF PARTICLE SOURCE TERMS: \( S_{\phi,d} \)

velocity and \( \delta t_L \) is the Lagrangian time-step at which the parcel is stepped. \( \delta t_L \) is the smallest timescale relevant to the parcel movement. Defining the cell parcel timescale \( \delta t_c \) as the time taken to traverse a fraction \( C \) of a characteristic local cell dimension \( l_{cell} \):

\[
\delta t_c = C \frac{l_{cell}}{|\vec{u}_p|}
\]  

(4.37)

where \( C \) is referred to as the parcel Courant number, than \( \delta t_L \) can be written as:

\[
\delta t_L = \min[\delta t, \delta t_c, T_I]
\]  

(4.38)

where \( \delta t \) is the carrier phase time step for transient flow and \( T_I \) is the turbulent eddy interaction time, defined in equation (3.10).

4.6 Calculation of Particle Source Terms: \( S_{\phi,d} \)

Integrating the particle equations results in trajectories: series of time, parcel position, velocity, temperature and traversing cell identity number. The parcel source terms are \( S_{u_i,d} \), \( S_{T_i,d} \), \( S_{k,d} \) and \( S_{\phi,d} \). The \( S_{\phi,d} \)-field values in the steady-state analysis are determined by adding the parcel contributions \( S_{\phi,p} \)\(^1\) of every iteration and dividing by the number of iterations. This allows the changing of trajectories during iterations and provides a relaxation of the source terms towards their converged values. For transient analysis \( S_{\phi,d} \) is identical to \( S_{\phi,p} \).

\( (S_{u_i,p}) \)

The contribution of the parcels to the source term of a particular cell number is calculated by selecting all time-steps of parcels in a cell, evaluating the time-step averaged hydrodynamic interaction force and summing over all trajectories:

\[
(S_{u_i,p}) = \frac{1}{V_{cell}} \sum_{tracks} \frac{n_p}{n_{steps}} \sum_{n_{steps}} S^n_{u_i,p}
\]  

(4.39)

\[
S^n_{u_i,p} = m_p \frac{u^n_{i,p} - u^0_{i,p}}{\delta t_L} - F^n_{pi} - F^n_{bi,i}
\]  

(4.40)

Where \( n_p \) is the number of particles represented by the parcel, \( n_{steps} \) is the number of time-steps over which is averaged, \( S_{u_i,p} \) is the hydrodynamic force on a parcel during its time-step, \( m_p \) is the mass of a particle, \( \delta t_L \) is the difference between \( t^0 \) and \( t^n \), the times corresponding to \( u^0_{i,p} \) and \( u^n_{i,p} \). The contribution is divided by \( V_{cell} \), so that the field values can be interpolated to staggered velocity nodes and adapted to their control volume.

\(^1\)Notice the difference in subscript indexing of d to p.
CHAPTER 4. NUMERICAL ANALYSIS

\( \langle S_{c,T,p} \rangle \)

The contribution of the parcels to the source term of a particular cell number is calculated by selecting all time-steps of parcels in a cell, evaluating the time-step averaged heat flow and summing over all trajectories:

\[
\langle S_{c,T,p} \rangle = \frac{1}{V_{cell}} \sum_{tracks} \frac{n_p}{n_{steps}} \sum_{n_{steps}} \left( m_p \frac{c_{p,p} T_p^n - T_p^o}{\delta t_L} \right) \quad (4.41)
\]

Where \( c_{p,p} \) is the mass based heat capacity of the particle material and \( T_p \) is the parcel temperature.

\( \langle S_{k,p} \rangle \)

The contribution of the parcels is calculated as follows:

\[
\langle S_{k,p} \rangle = \frac{1}{V_{cell}} \sum_{tracks} \frac{n_p}{n_{steps}} \sum_{n_{steps}} (u_{i,p}^n s_{u_i,p}^n) - \langle u_{i,f} \rangle \langle S_{u_i,p} \rangle \quad (4.42)
\]

\( \langle S_{e,p} \rangle \)

The contribution of the parcels is calculated as follows:

\[
\langle S_{e,p} \rangle = C_e \frac{\epsilon}{K} \langle S_{k,p} \rangle \quad (4.44)
\]
Chapter 5

Star CD’s Implementation

Star-CD’s setup of two-phase flow is not identical to the equations derived in the previous chapters. Main difference(s)

- for one-phase flow is the thermal energy equation,
- for two-phase flow are the position in the equations of the continuous phase volume fraction $\alpha_c$ and the absence of phase-interaction source terms in the $k-\varepsilon$ model equations,
- for the discretized equations are the collocated grid arrangement and the adaptation of the algebraic relations to non-orthogonal meshing,
- and for the algorithms is the adaptation of PISO with an undetermined number of corrector stage.

In the first section the forces implemented in Star-CD and the coupling deviating from the previous chapters are treated. The other differences in implementation are treated in the same order as above in the itemization. In appendix C the Star-CD equations are compared to the equations given by Gouesbet [18] and Crowe [23].

5.1 Implemented Forces and Coupling

Star-CD has implemented added mass-, drag-, gravity- and pressure-force. The pressure force is defined as in equations (3.14)-(3.15). Star-CD has a turbulent dispersion switch for a eddy-life-time-like model. The model deviates from the one described in section 3.2.1 only with respect to the times taken into account for assessment of the Lagrangian time-step. All models in relation to the particle equations contribute characteristic times, which minimum determines the Lagrangian time step. Only the drag- and added-mass-force contribute to the hydrodynamic interaction. The change in momentum of the parcel minus the pressure-force and body-forces is therefore equal to the interaction force and is the formulation of the momentum coupling term.

In the Star-CD manual is written that nothing but body forces may be implemented using the user-coded subroutine DROMOM.F. Therefore the transverse lift force, a
hydrodynamic interaction force, will be implemented as a body-force, resulting in a
change of parcel trajectory, but not in a change of momentum coupling. Use of the
transverse lift force is therefore restricted to very dilute flow.
Star-CD methodology states that no $k$-$\varepsilon$ coupling terms are provided, since no model
has been established for it. User-programming is made available through source term
definition in SORKEP.F.

5.2 Different Formulation of the Thermal Energy Source
Term

The difference between both terms is:

\[
\text{Chapter 2} \quad \frac{\partial u_i \tau_{ij}}{\partial x_j} \quad \text{Star-CD} \quad \tau_{ij} \frac{\partial u_i}{\partial x_j}
\]

The reason for this difference is that Star-CD derives the thermal energy balance
by subtracting the kinetic energy from the total energy balance. The source term
in the total energy balance is identical to the term in the thermal energy balance
of equation (2.16). The term $\tau_{ij} \frac{\partial u_i}{\partial x_j}$ represents the irreversible conversion of kinetic
energy into internal energy. The reason for the use of the total energy source terms
is the formulation of the thermal energy balance from a balance over a box of finite
dimensions.

5.3 $\alpha_c$ Positioning in Momentum Equation

Star-CD adapts its one-phase equations to two-phase equations by changing $\rho_c$, $\mu_{eff}$
and $S_\phi$ to respectively $\alpha_c \rho_c$ and $\alpha_c \mu_{eff}$ and $\alpha_c S_\phi$. Using $F_{p,t} = V_p \frac{\partial \rho}{\partial x_i}$ the $\alpha_d \frac{\partial \tau_{ij}}{\partial x_j}$
term of equation (3.52) vanishes, resulting in the vanishing of the $\alpha_c$ term before
the molecular diffusion term in equation (3.53). The resulting diffusion terms and
the terms implemented by Star-CD deviate:

\[
\text{Chapter 3} \quad \frac{\partial}{\partial x_j} \left( \mu \frac{\partial u_i}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left( \alpha_c \mu_{eff} \frac{\partial u_i}{\partial x_j} \right) \quad \text{Star-CD} \quad \frac{\partial}{\partial x_j} \left( \alpha_c \mu_{eff} \frac{\partial u_i}{\partial x_j} \right)
\]

Where $\mu_{eff} = \mu + \mu_t$. This discrepancy is unimportant for highly turbulent flow,
where $\mu_t \gg \mu$. It can be important for confined flow near the walls, where $\mu_t \approx \mu$
and the first term cannot be neglected.

5.4 Algebraic Relations

Star-CD approximates the diffusion term $B$ by face-centered expressions of the form:

\[
B \approx \sum_k \Gamma_{\phi,k} \left[ f_k^l (\phi_K - \phi_P) + \left( \text{grad} \phi \cdot \bar{S} - f_k^l \text{grad} \phi \cdot \bar{d}_{PK} \right) \right]
\]  
(5.1)
5.5. PISO

Where the first term in the brackets represents the normal diffusion between P and a neighbor cell centered node K and the second term within the curly brackets is the cross-diffusion. The terms $f^d_k$ are geometrical factors, $\vec{d}_{PK}$ is the distance vector between P and K, $\tilde{S}$ is the interface between the cells. When $f^d_k$ is identified with $A_k/\delta x_k$, then the difference between the derived B-term 4.9 and Star-CD is the cross-diffusion term.

Star-CD uses a collocated variable arrangement with cell centered nodal values. The face velocities $u_k$ need to be expressed in terms of the nodal velocities and neighboring pressures, for example $u_e$:

$$\overline{A_P}u_{i,e}^n = \sum_m A_m u_{i,m}^n + \left(\frac{\rho V}{\delta t} - u_{i,p}^o + \tilde{s}_1 + D_p (p_p^n - p_E^n)\right)$$

(5.2)

Where the over-bars denote 'a form of averaging' on the nodal momentum coefficients appearing under them, $m$ are 'all neighboring nodes used', $u_{i,m}$ are the nodal velocity-components, $\delta t$ is the transient time step, which is infinity for steady-state, $s_1$ is the source term, a function of 'the nodal velocity fields $u_i^o$, $u_i^p$ and other quantities' and $D_p$ is a geometric coefficient.

Even while Star-CD’s explanation is somewhat vague, it seems safe to assume that Star-CD saves memory space, by not needing to allocate the positions of the staggered grid nodes, at the cost of computational power by evaluation of the interface velocities and the nodal velocities.

Substituting the last equation into the continuity equation yields a pressure equation:

$$A_{pp}^n = \sum_m A_m p_{m}^n + s_1^n$$

(5.3)

5.5 PISO

Star-CD’s PISO implementation deviates on three points from Versteeg [26]. First it solves the nodal velocity field $u_i$ and calculates the face velocities $u_{i,k}$ from it. Second it solves a p-field, instead of a pressure correction field. And finally the number of corrector stages is not predetermined; rather, it is judged from an internal measure of the splitting error. This would enhance the accuracy and reliability of the algorithm and would be necessary if the scalar fields are strongly coupled to the flow.

If the scalars are strongly coupled to the flow field through, for example compressibility effects or combustion, they are embedded in the main predictor/corrector sequence. Whether this means that you should switch compressible flow on even for water or that there is a build-in measure for coupling is not stated.
Chapter 6

Simulation Results and Discussion

6.1 Introduction

The simulation results are based on a vertical channel flow case and a vertical pipe flow case. These will be introduced in section 6.2. Section 6.3 treats mesh creation for two-phase flow in Star-CD. Due to the numerous problems encountered, this section is rather large in comparison with the others. In section 6.4 Star-CD's performance is tested using the experimental results of Stojanovic [14]. Star-CD's one-phase simulations agree well with the experimental data, but Star-CD's two-phase simulations do not agree at all. Due to absence of coupling between the dispersed phase and the \( k-e \) model equations, the \( k \)-centerline profile for dilute two-phase flow is identical to the one-phase flow centerline profile. Signorino's experimental results [16] for one-phase mixing are investigated in section 6.5 using the validated Star-CD one-phase flow simulation. Finally in section 6.6 the lack of effect of the implementation of the transverse lift force on the dispersed phase volume fraction field is treated.

6.2 Cases

In this section the experimental setup and results of Stojanovic [14] and Signorino [16] will be presented. Stojanovic works with dilute two-phase flow, while Signorino's experiment is a dense two-phase flow.

In dense two-phase flow, 4-way coupling, i.e. particle-particle interaction becomes important. Star-CD's collision model is based on O'Rourke's model and will work only for transient flow analysis. The case of Stojanovic is straightforward steady-state analysis using SIMPLE, with which Star-CD can be validated, while simulating Signorino calls for exploration of Star-CD's transient PISO algorithm. In the following subsections the cases are presented.
6.2.1 Stojanovic's Vertical Channel Flow

Stojanovic et al. [14] published a paper on turbulence modification in a dilute two-phase turbulent flow. The flow modelling is restricted to two-way coupling, with the emphasis on turbulence modulation due to particle presence. Turbulence is generated by a grid at the entrance of the channel, after which the turbulence decay is a function of the dissipation $\epsilon$ only [15]. Stojanovic's paper provides experimental values for $k$ at the centerline of the channel for a number of particle volume fractions and diameters. This allows for validation of the Star-CD code for one-phase and two-phase turbulent flow.

**Experimental Setup**

The experimental setup used is presented in figure 6.1. The details of the setup can be found in Geiss et al. [15]. The turbulent flow behind the turbulence generating grid (grid size $M=12\text{mm}$) approximates isotropic homogeneous turbulent flow. Mean velocity up to 12 m/s can be attained. The measurement section is designed as a vertical glass tunnel with inner dimensions of 0.2 m by 0.2 m by 2.0 m. Particles with diameters in the range from 120 - 480 $\mu\text{m}$ are used. Loading between 0 and 2 kg particle/kg air can be realized. Measurement equipment consists of a 2-D Phase-Doppler Anemometer (PDA) allowing for simultaneous measurement of mean velocities and higher moments for both phases, as well as particle diameters. Sending optics have a focal length equal to 310 mm and receiving optics equal to 400 mm. Particle concentration measurements are performed by conventional probe (patternator) techniques.

**Experimental Results**

Stojanovic reports four cases (see table 6.1), which show a turbulence attenuation for particle diameters of 120 $\mu\text{m}$ and a turbulence augmentation for diameters of 480 $\mu\text{m}$. The centerline $k$ profiles of the one-phase flow and the two-phase flow with a volume concentration of $8.5 \cdot 10^{-5}$ $\text{m}^3$ particles $\text{m}^{-3}$ are used for validation of Star-CD (see figure 6.2). Stojanovic showed that the dilute flow with small particles, which attenuate turbulence, can be simulated by using the standard terms as presented in section 3.4.1. He also showed that the augmentation of turbulence cannot be accounted for in simulations containing the standard terms (see figure 6.3).

6.2.2 Signorino's Vertical Pipe Flow

Signorino works on one- and dense two-phase pipe flow using temperature measurements of the mixing of two in temperature differing water streams. Assuming that the particles are small enough to be in thermal equilibrium with their surroundings\(^1\) if the resistance to heat transfer is located in the particles, than it can adapt to an instantaneous change of surface temperature in 1.7 ms ($Fo = at/d_p^2 = 0.1$). In Signorino's two-phase pipe...
Figure 6.1: Experimental setup of Stojanovic for two-phase flow. (a - blower, b - Venturi pipe, c - dosage sluice, d - contraction and turbulence generating grid, e - Phase Doppler Anemometer, f - cyclone, g - filter section)

Table 6.1: Cases reported by Stojanovic

<table>
<thead>
<tr>
<th>No. of phases</th>
<th>$d_p$</th>
<th>$\alpha_d$</th>
<th>$z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>120 (\mu m)</td>
<td>8.5 (\times 10^{-5})</td>
<td>1.8 (\times 10^{-4})</td>
</tr>
<tr>
<td>2</td>
<td>480 (\mu m)</td>
<td>4.1 (\times 10^{-4})</td>
<td>8.7 (\times 10^{-4})</td>
</tr>
</tbody>
</table>

Where $d_p$ is the particle diameter, $\alpha_d$ is the dispersed phase volume fraction and $z$ is the loading as defined in equation 3.31, assuming with Stojanovic that the dispersed phase initial velocity can be set at 90% of the initial continuous phase velocity.
Figure 6.2: Stojanovic's experimental results. Reprinted from [14]. Comparison of gas-phase turbulent kinetic energy $k$ in $m^2/s^2$ against non-dimensional distance $x/M$ in a single-phase flow and a 2-phase flow with $120 \mu m$ particles and volume-concentration equal to $8.5 \cdot 10^{-5}$. Notice the log-log scaling on the axes.
Figure 6.3: Stojanovic's experimental results. Reprinted from [14]. Turbulent kinetic energy $k$ in $m^2/s^2$ against non-dimensional distance $x/M$ along the centerline of a 2-phase flow with 480 $\mu m$ particles and a volume concentration equal to $4.1 \cdot 10^{-4}$. 
CHAPTER 6. SIMULATION RESULTS AND DISCUSSION

Table 6.2: Geometrical measures of Signorino’s pipe

<table>
<thead>
<tr>
<th>Geometrical Measure</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R_{\text{inner, glass pipe}}$</td>
<td>7.5 mm</td>
</tr>
<tr>
<td>$R_{\text{inner, iron pipe}}$</td>
<td>5.0 mm</td>
</tr>
<tr>
<td>$R_{\text{outer, iron pipe}}$</td>
<td>5.6 mm</td>
</tr>
<tr>
<td>$L_{\text{iron pipe}}$</td>
<td>10 cm</td>
</tr>
<tr>
<td>$L_{\text{glass pipe}}$</td>
<td>1.5 m</td>
</tr>
</tbody>
</table>

Due to the high concentration of particles, particle-particle interaction has to be taken into account.

Experimental Setup

Signorino uses two barrels filled with water or water/particles, which are kept at different temperatures. Using gravity the flows go down to a pipe, where they are mixed. It is assumed that there is no thermal energy loss during transport from storage barrel to pipe. The glass pipe is fitted with a smaller steel pipe, such that the cross-sectional area of the inner iron pipe and the annular region between the pipe and the inner wall of the glass are the same. The inner pipe extends 10 cm into the glass pipe, after which the mixing takes place. It is assumed that the glass pipe wall is adiabatic. The stream exiting the glass pipe is collected in a barrel. Geometrical measures are given in table 6.2. At different axial positions the temperature is measured for four radial positions. This is done intrusively using thermocouples which are fixed at a radial position on a cross. The cross extends from the center to the wall, with 1.2 mm thick legs, thereby blocking minimally 19.6% of the cross-section of the pipe.\(^2\)

The weight of the barrels is measured at the beginning and the end of an experiment and the flow to the pipe is controlled by valves. The reported velocities are averages over the time of the experiment.

The particles used for the two-phase experiment are glass beads with a density of 2350 $kg/m^3$, a heat capacity of 834 $J/(K kg)$ and a particle size distribution of:

$$P(d_p) = 0.044e^{-\frac{(dp-55)^2}{20^2}} + 0.32e^{-\frac{(dp-90)^2}{10.3^2}}$$ (6.1)

The simulation shows that with $\alpha_d = 0.01$ and $v_{\text{inlet}} = 2.78$ m/s, it takes 40.4 cm before all dimensionless liquid temperatures $|T_{\text{average}} - T|/(T_{\text{hot}} - T_{\text{cold}})$ are below 0.02, corresponding to a particle travel time $t_{\text{travel}} = 145$ ms. During its movement through the in temperature varying liquid, the particle can adapt 85 times. In the simulations the particle time step is controlled by $T_i = \min(T_R, T_E)$, where $T_R \geq 1.9$ ms and $T_E \geq 2.8$ ms. That means that within every time step thermal equilibrium is achieved. Both for experiment and simulation the assumption of thermal equilibrium seems justified.

\(^2\)The center of the cross is probably bigger than the legs alone, for accommodation of the iron rod on which the cross is placed.
Figure 6.4: Scheme of Signorino's experimental setup
CHAPTER 6. SIMULATION RESULTS AND DISCUSSION

**Particle Size Distribution**

Where \( P(d_p) \) in \( m^{-1} \) is the probability of a particle with diameter \( d_p \) in \( \mu m \). See figure 6.5 for the plot of \( P(d_p) \). This comes down to 21\% of the beads being normally distributed with a mean of 55 \( \mu m \) and a standard deviation of 20 \( \mu m \), and 79 \% of the beads being normally distributed with a mean of 90 \( \mu m \) and a standard deviation of 10.3 \( \mu m \).

**Experimental Results**

Two cases of Signorino are used. A single phase experiment and a two-phase experiment with a particle volume concentration of 0.01. The cold stream enters the pipe through the center, the hot stream through the annular region. See table 6.3 for the inlet temperatures. The experimental results are presented in figures 6.6 and 6.7.

Two preliminary remarks can be made. First the two-phase flow takes a greater distance to come within close range of the average temperature, than the one-phase flow. When ascribed to turbulent mixing, the intensity of turbulence is less when the particles are added. This results is in agreement with theory and Stojanovic’s results. Second the measuring device used is too intrusive for measurements closer than 2 cm to the mixing point [16], so the graphs start at 2 cm.
### Table 6.3: Inlet temperatures of Signorino’s experiments

<table>
<thead>
<tr>
<th>Type</th>
<th>Temperature 1</th>
<th>Temperature 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>one-phase</td>
<td>11.4°C</td>
<td>48°C</td>
</tr>
<tr>
<td>two-phase</td>
<td>16.8°C</td>
<td>55.6°C</td>
</tr>
</tbody>
</table>

![Temperature Profiles at Radial Positions](image)

**Figure 6.6:** Signorino’s experimental one-phase flow results. $T_{\text{hot}} = 48.0^\circ\text{C}$. $T_{\text{cold}} = 11.4^\circ\text{C}$. $v_{\text{in}} = 2.78 \text{ m/s}$. Measured temperatures at the above indicated radial distances from the center for a range of 2 - 50 cm distance from the mixing point.
Figure 6.7: Signorino's experimental two-phase flow with 0.01 volume concentration results. $T_{\text{hot}} = 55.6^\circ\text{C}$. $T_{\text{cold}} = 16.8^\circ\text{C}$. $v_{\text{in}} = 2.78\ m/s$. Measured temperatures at 4 radial distances from the center for a range of 2 - 50 cm distance from the mixing point.
6.3 Star-CD Mesh Creation

This section starts with an introduction to Star-CD mesh creation, followed by the meshes created for the two cases at hand. The channel mesh is a uniform mesh, build after the pipe mesh. Therefore no problems were encountered and the pages spend are small in comparison to the non-uniform pipe meshing.

6.3.1 Introduction

Star-CD makes use of a collocated grid with the velocity-components and the other scalars stored at the center of a cell. A cell is defined by its eight corner vertices. Creating a mesh in Star-CD entails the definition of vertices, from which directly or by use of mesh creation aids cells can be defined. Basic aids are the definition of a patch by four vertices, definition of a block by eight vertices and the definition of a spline by a range or a list of vertices.

Two basic routes lead to a three dimensional grid. A three dimensional block can be defined to have X cells in the x-direction, Y cells in the y-direction and Z cells in the z-direction. After that the block is executed: the needed cells and vertices are generated by Star-CD. Another way is to create a two dimensional area with X by Y shells by patching the area between four vertices. This two-dimensional area is than extruded in the coordinate direction normal to the surface into a number of cell layers. Block execution and extrusion can take place in any coordinate system, creating a three dimensional structure following that system. A Cartesian coordinate system results in rectangular cells, a cylindrical coordinate system results in cells shaped like parts of a circle with constant thickness and width and a spherical coordinate system results in cells shaped like parts of a four-sided spike, which has its tip in the center and its top corners are equidistant to the tip. See figure 6.8 for a representation of a spherical cell.

Different three dimensional structures can be defined in the same space leading to interfaces, which are doubly defined. When the vertices defining the cell surfaces are identical in position, they can be merged into one: deleting one set of vertices. When not identical, cell surfaces have to be coupled to the other surfaces using a master slave approach. A master surfaces faces a number of slave surfaces. This imposes a restriction on mesh formation, because for a cell face facing two different master cell faces, an arbitrary choice has to be made to which cell it is to be coupled. For the joining of a Cartesian and a cylindrical based surface the coupling is impossible or highly specialistic.

Figure 6.8: Representation of a spherical cell.
6.3.2 Channel Meshing

Stojanovic reports that he uses a collocated grid with an uniform mesh of 34X34X74 cells, creating a $0.2 \times 0.2 \times 2 \, m^3$ 3D flow structure. Following Stojanovic the cells are not refined near the walls. The two reasons for this are that only information about the centerline of the channel for the first 60 cm is needed, so the boundary layer is not expected to have grown thick enough and that wall refinement led to wall accumulation in the pipe flow (see section 6.3.3). The mesh is generated by defining the eight corner vertices of the channel, defining a block by these eight vertices and executing the block to generate the cells. The commands needed can be found in appendix D.1 under the heading Mesh generation. A top view of the mesh of the channel is presented in figure 6.9.

6.3.3 Pipe with Inlet Meshing

While Stojanovic's mesh is a block with geometrical dimensions thousand times larger than the particle diameter, Signorino's pipe is cylindrical with a diameter 15 times larger than the particles diameter. Eleven meshes have been designed, before a working design was found. They will be presented in the following paragraphs under the heading of the problem encountered.
6.3. STAR-CD MESH CREATION

Figure 6.10: Screen-shot of the 90° mesh. A quarter cut of the flow in the pipe with a free space for the steel inlet tube. In the corner are the 8 × 8 rectangular cells. After the mixing point the mesh is more refined in the axial direction.

Starting problem situation

Due to the expected problem of a singular point in the center of the pipe, two meshes were give by the TU-Berlin group, which circumvented this. A 90° cut of the pipe, where the center is formed by 8 × 8 rectangular cells. The other cells are generated within a cylindrical coordinate system. To this mesh is referred as 90°. A screen-shot of the 90° mesh is shown in figure 6.10. The sides of the 90° pipe-cut are treated as cyclic boundaries coupled to each other, assuming that the flow is symmetrical with the respect to the pipe’s inner angle $\theta$. The cubic center cells avoid the junction of all cylindrical slices at the center.

The other mesh is a 4° slice of the pipe, again with cyclic boundaries. The thinness of the slice allows one cell in the $\theta$ direction, so that one triangular cell is at the center. Thereby avoiding the connection of too much cells at the same point. To this mesh is referred as 4°. A screen-shot of the 4° mesh is shown in figure 6.11.

Star-CD calculates with Cartesian coordinates during simulation, and the Cartesian form of the transport equations. Hereby the problem of the radius approaching zero, c.q. the inverse of the radial coordinate approaching infinity is circumvented. Furthermore Star-CD is meant for use with non-uniform cells and it uses a collocated grid to reduce memory needed to store the extra nodal positions. The problems circumvented by the given meshes are general problems, which do not apply to Star-
Figure 6.11: Screen-shot of the 4° mesh. A 4° slice of the flow in the pipe with a free space for the steel inlet tube. The volume of the triangular cell in the corner is below the minimum cell volume for Lagrangian two-phase simulations with particle diameters in the order of 100 μm.
6.3. STAR-CD MESH CREATION

The given meshes have been developed in view of a staggered formulation of the numerical environment. Using a staggered grid for the velocity components, which nodal positions are placed on the interfaces of the cells, would lead to one velocity components nodal position at the center. This occurs when multiple triangular tips come together in the center, the normal occurrence for a cylindrical designed mesh. This nodal position would then occur in more than two sets of algebraic relations, thereby overdefining it. This could be a problem for iterative calculations.

When the algebraic relations are derived for non-uniform cells, geometric constants are included, such as the surface area. Since the surface area for the center node is zero, the value of the node would not matter and no problem could be encountered. When a collocational grid is used, which stores the velocity components at the same nodal positions as the scalar values, no node is found at the center and no problem would be encountered.

Mesh creation in Star-CD is thus not restricted by the problem of a singular point in the center of the pipe.

Minimum cell volume

Simulations of two-phase flow using Lagrangian analysis with the given meshes poses the problem of minimum cell volume. From error-messages it became clear that Star-CD poses a limit of 0.40 to the dispersed phase volume fraction for Lagrangian two-phase analysis. When all parcels present in a cell occupy more than a volume-fraction of 0.4 Star-CD generates an error message and sets the dispersed phase volume fraction $\alpha_d$ to 0.40.

When a parcel of particles is in a cell it occupies a volume $V_p$ of $\frac{\pi}{6}d_p^3n_p$. For steady-state analysis the dispersed phase volume fraction $\alpha_d$ is calculated by first summing over all parcel-volumes in a cell $\sum_k \frac{\pi}{6}d_p^3n_{p,k}/V_{cell}$, where $k$ is the summing index. Then the values for each cell are averaged over all iterations. The averaging over all iterations allows the change of parcel trajectories during iterations, due to the random turbulent dispersion or change of initial position and lets $\alpha_d$ approach its steady-state value gradually.

When $\frac{\pi}{6}d_p^3n_p/V_{cell, min}$ is larger than 0.4 errors will be generated during the first iteration(s) of steady-state analysis, averaging out in later iterations, due to iterations where the calculated $\alpha_d$ is zero, due to the absence of parcel tracks through the cell.

For transient analysis errors will be generated during every time step in which the calculated dispersed phase volume fraction is above 0.4. Because of the possibility of multiple parcels being present in one cell the minimum cell volume in a transient two-phase Lagrangian analysis has to be a multiple of $V_pn_p/0.40$. Both meshes fail

For transient analysis $n_p$ is the number of particles per parcel, which is effected by the initial setting and collisions. For steady-state analysis $n_p = \dot{n}_p \Delta t_{cell}$, where $\dot{n}_p$ is the particle number flow and $\Delta t_{cell}$ is the time it would take to traverse the cell. This time can be calculated on basis of the trajectory information.
CHAPTER 6. SIMULATION RESULTS AND DISCUSSION

Table 6.4: Minimum cell volume and one particle volume fraction

<table>
<thead>
<tr>
<th>Cell Angle (°)</th>
<th>( V_{\text{cell}, \text{min}} ) (( 10^{-12} \text{m}^3 ))</th>
<th>( \frac{V_p}{V_{\text{cell}, \text{min}}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>4°</td>
<td>( 4.1 \cdot 10^{-12} \text{m}^3 )</td>
<td>0.47</td>
</tr>
<tr>
<td>90°</td>
<td>( 6.6 \cdot 10^{-12} \text{m}^3 )</td>
<td>0.29</td>
</tr>
</tbody>
</table>

All simulations are steady-state with \( v_\text{in} = 2 \text{ m/s} \), \( d_p = 100 \mu \text{m} \). Minimum cell volumes are located at the tip for the 4° slice and at the center for the 90° pipe cut.

This criterion for a particle diameter of 100 \( \mu \text{m} \) (see table 6.4). The number of particles a parcel represents is limited to the computational power available. How smaller this number, the better the spreading of the parcels over the domain, giving a lower chance of locally crossing the 0.40 fraction.

Star-CD also generates errors when the ratios of the cell dimensions exceed the factor 10. This is justified by the argument that the z-velocity component is in the order of 1 m/s, while the x- and y-components are more than two orders lower. Hence the non-dimensionalized cell dimensions \( \Delta z/(v_z \tau) \approx \Delta x/(v_x \tau) \approx \Delta y/(v_y \tau) \), are approximately the same and their ratios are of order 1.

A new 90° pipe-cut mesh is designed in which the small \( 8 \times 8 \) center cells are replaced by \( 2 \times 2 \) cells. To this mesh is referred as \( 90° (2 \times 2) \). A screen-shot of the \( 90° (2 \times 2) \) mesh is shown in figure 6.12. This coarsening of the center replaces the problem of too small cells with the problem of multiple slave cell-faces facing one master cell-face. The 16 cylindrical cell faces, which were merged with the inner \( 2 \times 8 \) cell faces of the center cube, are chosen to be coupled as two slaves to one master cell face. Therefore a transitional layer of \( 2 \times 4 \) cells was placed between the 16 cylindrical cell faces and the \( 2 \times 2 \) core. This resulted in two oddly shaped cells in this transition layer with faces on the 45° line.

The minimum cell volume of the new \( 90° (2 \times 2) \) is \( V_{\text{cell}, \text{min}, 90° (2 \times 2)} = 9.5 \cdot 10^{-11} \text{m}^3 \) and these cells are the cylindrical cells placed at the outer rim.

To minimize the possibility of multiple parcels in the same cell the initial parcel positions are no longer the same for each steady-state iteration or transient time step, but are randomly calculated positions within the inlet area. To this purpose the user-code DROICO.F is adapted (see E.1).

A Lagrangian analysis is physical acceptable only [6] when the cell dimensions are a factor 3 greater than the particle diameter. The minimal distance between vertices is \( d_{\text{vertex, min}} = 170 \mu \text{m} \), making a \( d_p = 57 \mu \text{m} \) acceptable. The average vertex distance is large enough to accept a simulation with \( d_p = 100 \mu \text{m} \).

\(^4\tau\) is the space time \( L_{\text{pipe}}/(v) \) and \( L_{\text{pipe}} \) is the length of the pipe.
Figure 6.12: Screen-shot of the 90°(2 × 2) mesh. A quarter cut of the flow in the pipe with a free space for the steel inlet tube. In the corner are the 2 × 2 rectangular cells, coupled in a ration of 1:2 to the layer of oddly shaped cells, which are coupled in a ration of 1:2 to the next layer. The mesh is refined in the axial direction towards the mixing point.
High turbulence area at the mixing zone

One-phase simulation results of this new grid failed to represent the high turbulent kinetic energy area, which should be present at the mixing zone. Refining the mixing-zone would be a first approach to resolve $k$ far enough to get the $k$-spot. Because of the large increase in the number of cells for the refinement of the mixing zone in the 90° cut the choice is made to refine the 4° slice. The 4° slice is refined in the mixing zone and coarsened in the tip. This results in a minimal cell volume of $V_{cell,min,4°-refined} = 21 \cdot 10^{-11}\text{m}^3$ for cells in the mixing zone. To this mesh is referred as 4°-refined.

Using the second order accurate differential scheme QUICK the $k$-spot could be resolved. But the temperature field of the simulation exhibited a low temperature spot with temperatures below the cold inlet temperature. Figure 6.13 shows contour-plots of the temperature field with the T-spot. Due to further changes to the mesh and loss of simulation data, the $k$-spot cannot be shown. QUICK is known to retain oscillations, resulting in such spots. Therefore the MARS scheme is used, which is also second order accurate, but has a build-in oscillations dampener. The formulation of the scheme is not given by Star-CD.

The simulation with the MARS scheme resulted in the absence of both the low temperature spot and the high turbulent kinetic energy spot. Because nowhere in the previous simulations with Star-CD nor with Dr. Varone's personal code the high turbulent kinetic energy spot was resolved this issue has been abandoned. Nowhere in the simulations is a clear high turbulent kinetic energy spot to be found.

From this point onward the temperature dependence of the viscosity of water will be accounted for by a polynomial, which is implemented in the user-code VISMOLF (see E.4). The reason for implementation is that in the annular region the flow is laminar when the viscosity of the cold inlet temperature is used ($Re_{11°C} \approx 10^3$), while it is turbulent when the temperature of the hot inlet temperature is used ($Re_{56°C} \approx 2.6 \cdot 10^3$). Signorino has already found the same result experimentally. The experimental setup would only work, when the hot stream was in the annular region between the outer pipe wall and the inlet-pipe.

Wall parcel accumulation

In Star-CD evaluation of the turbulent kinetic energy $k$ near walls can be done using wall-functions or the 2-layer model. The wall-function uses the center of the cells adjacent to the wall as $y^+$ value and calculates $k$-values between wall and center using a function in which $y^+$ is used to normalize the wall distance. For the other half of the cell the transport equations are used. The turbulent dissipation $\epsilon$ is evaluated in both regions with the transport equations. The 2-layer model calculates within a specified wall distance whether to use a function or the transport equation for $k$. This results in a less mesh dependent switch between function and transport equation calculation of $k$.

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5The mixing zone is where the inner pipe vanishes and the streamlines change to fill the gap.
6.3. STAR-CD MESH CREATION

(a) The contour-lines bend upwards at the wall, due to the 2-layer model with a 2-layer thickness of 600 μm. Increasing the 2-layer region to 1200 μm makes the bend more pronounced, switching to wall-function makes the bend disappear. On the center-side of the steel-pipe vacancy is a cold-spot.

(b) Detail of the contour-plot. The cold-spot is lower in temperature than the inlet temperature.

Figure 6.13: Contour lines plots of the T-field in the 4°-refined mesh using the QUICK differencing scheme for the thermal energy equation and 2-layer model for the turbulent energy $k$ wall treatment.
CHAPTER 6. SIMULATION RESULTS AND DISCUSSION

<table>
<thead>
<tr>
<th></th>
<th>$\alpha_{d,in}$</th>
<th>$\alpha_{d,max}$</th>
<th>$\alpha_{d,min}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-Layer</td>
<td>0.03</td>
<td>0.22</td>
<td>0.002</td>
</tr>
<tr>
<td>2-Layer</td>
<td>0.04</td>
<td>0.33</td>
<td>0.0025</td>
</tr>
<tr>
<td>Wall function</td>
<td>0.03</td>
<td>0.061</td>
<td>0.0024</td>
</tr>
</tbody>
</table>

All simulations are steady-state with $v_{in} = 2 \text{ m/s}$, $d_p = 100 \mu\text{m}$. Minima are located at the inner side of the inlet pipe. Maxima are found at the wall, 50 cm from the mixing point.

Maciocco et al. [27] did an analysis on the effects of Star-CD’s options on simulation results for standard flow cases, such as the backward facing step. One of their results is that even for non-refined wall areas the 2-layer model gives better results than the wall-function for the evaluation of the turbulent kinetic energy $k$. Because the vanishing inner pipe can be seen as two piggy-backed backward facing steps, this is a reason to implement the 2-layer model.

A $5^\circ$ mesh is designed with wall refinement at the inner and outer pipe for use with the 2-layer model. To increase the cell volume of the refined wall cells the slice angle is increased to $5^\circ$. To this mesh is referred as the $5^\circ$. The commands needed to generate this mesh can be found in appendix D.3. The cells adjacent to the wall are approximately $100 \mu\text{m}$, thereby violating the criterion of a factor 3 difference between cell dimensions and a particle diameter of $100 \mu\text{m}$.

Maciocco et al. only investigated the effect on the velocity components, $k$ and $\epsilon$ in one-phase flow. Including temperature shows a strange curvature of the temperature profiles in the laminar part of the 2-layer model, bending slightly downstream, implying slower mixing in the laminar wall region. See figure 6.13a for the effect in the $4^\circ$-refined mesh for a 2-layer region, which extents to $600 \mu\text{m}$ off the walls.

Simulating steady-state two-phase flow with a volume fraction of 0.03 and $100 \mu\text{m}$ particles resulted in dispersed phase volume fractions up to 0.22 for the cells at the wall. Switching to the wall-function resulted in a reduction of the volume fraction up to 0.06 at the wall. See table 6.5 for simulation specifications. Even while the criterium of a factor 3 difference between cell and particle dimensions is violated, there is no reason to assume that smaller particles would have resulted in no wall accumulation.

The explanation for the results is the Star-CD particle-wall collision treatment. Because the particles are taken as point-particles representing a cluster of particles, the parcel-wall collision is resolved when the mass-center is at the wall, instead of at a distance equal to the radius of the parcel. The parcel traverses into the laminar region, in which the turbulent dispersion is insignificant and the drag coefficient is larger and gets stuck. Switching to the wall-function reduces the laminar region to only one half of the cells, while the 2-layer model assigned two whole cells adjacent to the wall.

Coarsening the wall region and using the wall function got rid of all wall accumulations. Accumulation being arbitrarily defined as a cell in which the dispersed phase volume fraction is more than 150 % of the inlet volume fractions.
Center parcel accumulation

Getting rid of the 6.1 % wall volume percentage by coarsening the grid, made the center accumulation, which also amounted to 6.1 % with a inlet volume percentage of 3 %, also suspect of being numerical in nature. Visualization of the particle tracks (see figure 6.14 a) showed a close proximity of subsequent parcel positions within a trajectory only found near the center of the slice.

A 25° slice of the pipe was created by extruding 5 slices of 5°. The same set of commands as for the 5° are needed (see appendix D.3). Simulations with the same parameters also gave a center accumulation. Track visualization showed the same close proximity pattern near the center (see figure 6.14 b), but the largest radial position at which the patterns start, has moved nearer to the center. Simulations with the 90° × 120° (10 × 10) mesh, which will be presented in Final mesh, showed no center accumulation.

The explanation for these result is the Star-CD’s cyclic boundary parcel crossing treatment. When the cyclic boundaries are too close to each other the parcels get stuck, causing a center accumulation. When the angle between the boundaries is increased five fold, the radial position at which it happens decreases nearly five-fold, implying that the boundary-boundary distance is crucial. Visualizations also showed parcel-trajectory positions with a negative radial positions, viz. outside the domain. Star-CD probably uses a truncation for the parcel movement through the cyclic boundary, in which a multiple of boundary-boundary distance is truncated, positioning the parcel at the effective position between the boundaries. With these small distances this could cause the almost neglectable parcel movement and the negative radial coordinate anomalies.

Coupled non-uniformly shaped cells

Due to the introduction of Signorino’s present experimental setup, the meshes had to be rescaled, thereby doubling their radial coordinates. Having abandoned the resolvement of high kinetic turbulent energy spots in the mixing zone and leaving the slices, because of their center accumulation, the 90° (2 × 2) mesh is scaled up to the measures as presented in table 6.2.

Steady-state simulation with this mesh led to an oscillation in the residuals of mass, \( A \) and \( e \). The following fruitless attempts were made to make the simulation converge. The relaxation factors of the velocity components and \( k \) and \( \epsilon \) were reduced from 0.7 to 0.4. The relaxation factor of pressure was reduced from 0.3 to 0.2. All Upwind differencing schemes were used. No parcels were introduced. Temperature effect was turned off.

The only complex feature of this mesh is the coupling of non-uniformly shaped cells in the layer between the center 4 rectangular cells and the cells, generated by executing a cylindrical coordinate system based block. (See figure 6.12.) The basic problem with Star-CD’s coupling of different parts of the mesh is due to cracks
between the parts. If two blocks face each other bounded by a spline, where the number of cells adjacent to the boundary is unequal, then the execution of those blocks will generate cracks, due to the different approximation of the spline by the cells generated. See figure 6.15. These cracks are a main problem when assigning master-slave couples. In the Star-CD manual coupling of a cylindrical with a Cartesian mesh is showed in z-direction only. This coupling doesn’t generate cracks, but our r-direction coupling does.

The only explanation for the oscillations in the residuals are the oddly shaped cells in the transitional layer at the 45° line in combination with coupling. Now that all surfaces normal to the radial-coordinate have increased four-fold, the coupling of the non-uniform shaped cells seems to generate the oscillations.

Final mesh

Keeping the idea of the center cells being Cartesian in nature, the small tips of cylindrical slices are avoided. Because in the slices the cell dimensions fall to zero, thereby violating the criterion stating that the cell dimensions should always be a factor 3 greater than the particle diameter. To avoid the problem of non-uniform cell coupling the inner Cartesian cells are generated by creating a block with an inner angle of 120°, which is coupled to the cylindrical blocks. The block consists of 10 × 10 cells, the cylindrical blocks consist of 2 × 10 slices, which are coupled to the Cartesian cell faces on a basis of 1 master to 1 slave. To this mesh is referred as $90° \times 120° (10 \times 10)$ (see figure 6.16). The commands needed to generate this mesh and its more coarse varieties can be found in appendix D.4. Star-CD gives no error messages up to a dispersed phase volume-fraction of 0.156, using 20,000
parcels to ensure a mass residual of $10^{-4}$. Star-CD calculates the dispersed phase volume fraction of a cell directly from the number of parcels in a cell. The high number of parcels is needed to keep the dispersed phase volume fraction constant.

Because Dr. Alberto Varone used the steady-state flow field calculated with Star-CD in his code it is requested to make a mesh with as little as cells as needed. To study the effect of mesh coarsening the $90^\circ \times 120^\circ$ mesh is also made based on 8 cells and based on 5 cells, giving the $90^\circ \times 120^\circ (8 \times 8)$ and $90^\circ \times 120^\circ (5 \times 5)$ meshes. Coarsening the grid makes field resolving faster at the expense of more iterations needed for convergence and at the expense of more parcels that are needed for a low enough mass residual. When the simulation could not reach the mass residual of $10^{-4}$ it was terminated and continued with a higher number of parcels. The number $10^{-4}$ is arbitrary and used throughout all simulations. Results of the study can be found in table 6.6. Roughly speaking the calculation of one iteration of one-phase steady-state flow takes a few seconds, the calculation of 10,000 parcel tracks takes 100 seconds on an IRIX64. The number of iterations needed for the different meshes is dependent on the moment at which a higher number of parcels is introduced. Basic strategy is to get a converged one-phase field, add 2000 parcels until the mass residual is below a number of $10^{-2}$, use 10,000 parcels to reach $10^{-3}$ and use 20,000, 40,000 or 60,000, respectively using the $10 \times 10$, the $8 \times 8$ or the $5 \times 5$ mesh. Based on the simulations performed the $5 \times 5$ mesh needs too many iterations to converge, while the $8 \times 8$ mesh could be brought down to 15 hours using the right tactics. Without knowing these it took 112 hours for the $5 \times 5$ and 50 hours for the $8 \times 8$. The Star-CD settings used can be set by the commands found in the appendix D.5.
Figure 6.16: Screen-shots of the final 90° cut of the pipe

(a) Screen-shot of the 90° Mesh

(b) 75° × 120° × 75° × 90° angles
6.4 Simulation of Stojanovic’s Results: k

Stojanovic’s results are estimated from the graph using a ruler. The one-phase k-values are taken from the normal-normal scaled graph as shown in figure 6.3 and from the log-log scaled graph of figure 6.2. The one-phase sets deviate at 12 and 36 cm from the grid. See figure 6.17. Based on theory one would expect that if the particles dissipate turbulence, that then a higher volume fraction would have a higher turbulence dissipation. But at distances 12, 18 and 36 cm from the grid the 4.2 $\times$ 10^{-5} volume fraction has a lower value for k than the 8.5 $\times$ 10^{-5} volume fraction. The difference between the two 2-phase sets is smaller than the difference between the 1-phase sets and can be accounted for as being within the ruler-graph estimation error $\text{graph} = 0.05 \text{ m}^2/\text{s}^2$.

One-phase grid generated turbulence decay

The commands for setup of Stojanovic’s channel flow in Star-CD can be found in appendix D.2. The simulations are performed with $k_{in} = 0.735 \text{ m}^2/\text{s}^2$, the experimental k-value at 12 cm from the turbulence generating grid taken from figure 6.3. With the inlet velocity set at 10 m/s in the axial direction, the only free variable is the inlet turbulent energy dissipation $\epsilon_{in}$. Simulations with $\epsilon_{in}$ values ranging from 0.02 to 500 $\text{m}^2/\text{s}^3$ are performed. They result respectively in a centerline k-profile as a straight declining line and as a line falling directly to almost zero and staying there. The $\epsilon_{in}$ values corresponding most with Stojanovic’s experimental results are 90, 100 and 110 $\text{m}^2/\text{s}^3$. A simulation using Chen’s $k - \epsilon$ model instead of the standard model only resulted in changes in the third digit behind the decimal point. As can be seen in figure 6.18, in which $k$ is non-dimensionalized with $k_{in}$ and the distance from the turbulence generating grid is in meters, at 24 cm from the grid the ‘experimental value’ is lower than the three simulation values, while at 60 cm it is the other way around. Comparing the non-dimensionalized simulation values with the second set of ‘experimental values’ with $k_{in} = 0.685 \text{ m}^2/\text{s}^2$ gets rid of the

Table 6.6: Effect of mesh coarsening on CPU-time and mass residual

<table>
<thead>
<tr>
<th>$\alpha_d$</th>
<th>$\bar{n}_p$</th>
<th>Mass Residual</th>
<th>Iter.</th>
</tr>
</thead>
<tbody>
<tr>
<td>90° x 120°(10 x 10)</td>
<td>0</td>
<td>&lt; 10^{-4}</td>
<td>3.84</td>
</tr>
<tr>
<td>90° x 120°(8 x 8)</td>
<td>0.10</td>
<td>20,000</td>
<td>&lt; 10^{-4}</td>
</tr>
<tr>
<td>90° x 120°(5 x 5)</td>
<td>0.10</td>
<td>10,000</td>
<td>1.94 $\times$ 10^{-4}</td>
</tr>
<tr>
<td>90° x 120°(5 x 5)</td>
<td>0.10</td>
<td>40,000</td>
<td>9.96 $\times$ 10^{-5}</td>
</tr>
<tr>
<td>90° x 120°(5 x 5)</td>
<td>0.10</td>
<td>40,000</td>
<td>1.09 $\times$ 10^{-4}</td>
</tr>
<tr>
<td>90° x 120°(5 x 5)</td>
<td>0.10</td>
<td>60,000</td>
<td>9.59 $\times$ 10^{-5}</td>
</tr>
</tbody>
</table>

Where $\alpha_d$ is the dispersed phase volume fraction, $\bar{n}_p$ is the particle number flow and the IRIX64 CPU-time is given in seconds per iteration.
CHAPTER 6. SIMULATION RESULTS AND DISCUSSION

Comparison of the $k$-values: graph-based

Figure 6.17: Estimated values for 1-phase channel flow and 2-phase flow with a $d_p = 120\mu m$ and a dispersed phase volume fraction of $4.2 \cdot 10^{-5}$ and of $8.5 \cdot 10^{-5}$. The mesh diameter of the turbulence generating grid $M=12 \text{ mm}$. 

- Gas- taken from fig.2 of Stojanovic's article
- Gas-solids $4.2E-5$, $120 \text{ mu}$
- Gas- taken from fig. 6 of Stojanovic's article
- Gas-solids $8.5E-5$, $120 \text{ mu}$
6.4. SIMULATION OF STOJANOVIC’S RESULTS: $k$

Figure 6.18: Graph of turbulence decay in 1-phase channel flow. The graph results of figure 2 in Stojanovic’s article are presented together with results of k-ε simulation using $\epsilon_{in}$ values of 90, 100 and 110 $m^2/s^3$ and with results of a k-ε Chen simulation using an $\epsilon_{in}$ value of 110 $m^2/s^3$. Vertical is $k/k_{in}$, horizontal is the distance from the turbulence generating mesh. $k_{in} = 0.735 m^2/s^3$ for all profiles.

Discrepancy at 24 cm, but is still a bit higher at 60 cm. $\epsilon_{in} = 100 m^2/s^3$ is chosen as the best value in which the simulation represents the experimental values. Defining the turbulent length scale $l$ as

$$l = C_l^{3/4} k^{3/2} / \epsilon,$$

(l becomes $10.4 mm$ at $x/M=10$. This is a bit smaller than the mesh diameter $M = 12 mm$ of the turbulence generating grid at $x/M=0$).

Two-phase grid generated turbulence decay

Simulations for two-phase flow are set up using the $k_{in}$-values as shown in table 6.7. As suggested by Stojanovic the initial parcel velocity is set at 90% of the gas velocity and 20,000 parcels are used. First a one-phase simulation is performed to

---

6The difference between the experimental sets at 24 cm is due to the non-dimensionalization with the first value of the sets and the error hereby introduced.
Figure 6.19: Graph of turbulence decay in 1-phase channel flow. Contrary to figure 6.18 the graph results of figure 6 in Stojanovic’s article (see figure 6.2) are used. Simulation profiles are the same as in figure 6.18. $k_{in}$ value for Stojanovic’s results is $0.685 \text{m}^2/\text{s}^3$.

Table 6.7: Simulation setup of Stojanovic’s two-phase experiments

<table>
<thead>
<tr>
<th>$d_p$</th>
<th>$\alpha_d$</th>
<th>$k_{in}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>480$\mu$m</td>
<td>4.1 $\cdot$ $10^{-4}$</td>
<td>1.7 $\text{m}^2/\text{s}^3$</td>
</tr>
<tr>
<td>120$\mu$m</td>
<td>4.2 $\cdot$ $10^{-5}$</td>
<td>0.555 $\text{m}^2/\text{s}^3$</td>
</tr>
</tbody>
</table>

Where $d_p$ is the particle diameter, $\alpha_d$ is the dispersed phase volume fraction and $k_{in}$ is the inlet turbulent energy. Values are taken from Stojanovic’s [14] plots of the experimental values at $x/M=10$. 
serve as an initial field for the Lagrangian two-phase simulation. After that parcels are initialized. There is no difference between the centerline k-profiles of the initial fields and the two-phase fields. Not even a qualitative correspondence between the centerline k-profiles for the 480 μm is found. In Star-CD version 3.15 the initialization and tracking of parcels has no effect on turbulence. The explanation for this is that there is no two-way coupling between the parcels and the k-ε model equations. The effect of parcels on the velocity components due to two-way coupling does not work through on k.

Implementation of a coupling by introducing a k source-term and an ε source-term in their transport equations can be done in Star-CD using the user-code SORKEP.F and implementing the $S_{k,d}$ and $S_{ε,d}$ terms (see equation 3.110 and 3.104). For calculation of these terms the trajectory information from the track file (case_name.trk, generated by Star-CD during every iteration,) has to be accessed. While this is possible with a stand-alone program using an old track file, this is not possible from a Star-CD user-coded subroutine. This problem has led to an extensive email correspondence with the Star-CD support, however not to a solution. The program which reads the track-file can be found in appendix F.1.

Since no other access to the trajectory information is available, no k-ε source terms can be evaluated, therefore no Lagrangian two-phase simulation can be performed with Star-CD.

### 6.5 Simulation of Signorino’s Results: T

Because Signorino experiments with dense two-phase flow, particle-particle interaction cannot be neglected. Star-CD has implemented O’Rourke’s collision model, which is only applicable to transient analysis. Therefore this section will begin with the problems encountered in Star-CD’s transient analysis, after which the results of the simulation of one-phase flow temperature profiles are presented.

#### 6.5.1 Transient scalar equations errors

The reason why collision modelling is restricted to transient analysis is that in transient analysis all parcels are stepped at the same time, thereby changing their position and velocity under effect of the presence of other parcels. While steady-state Lagrangian analysis reduces computational load by sequentially tracking the parcels through the fluid until exit or depletion. No collision can occur, while the presence of other particle tracks depends on the order of calculation.

O’Rourke’s model computes whether parcels in the same cell collide or separate, and whether there is subsequent coalescence or collision. This is done by checking whether a randomly generated number is lower than a calculated characteristic number for each event. For hard spheres no coalescence should occur. O’Rourke’s calculated numbers are only dependent on the Weber number, which is defined as [10]:

$$W_e = \frac{\rho_p |\bar{u}_f - \bar{u}_d| d_p}{2\sigma}$$  \hspace{1cm} (6.3)
Table 6.8: Effect of PISO pressure underrelaxation

<table>
<thead>
<tr>
<th>( f_{p-relax} )</th>
<th>( n_{steps} )</th>
<th>NSP</th>
<th>NPCOR</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.9</td>
<td>7</td>
<td>1600-10^4</td>
<td>6-66</td>
</tr>
<tr>
<td>0.7</td>
<td>3</td>
<td>2600-10^4</td>
<td>3-9</td>
</tr>
<tr>
<td>0.3</td>
<td>6</td>
<td>1400-4321</td>
<td>3-22</td>
</tr>
<tr>
<td>0.2</td>
<td>6</td>
<td>1565-3228</td>
<td>7-23</td>
</tr>
<tr>
<td>0.1</td>
<td>7</td>
<td>1625-3601</td>
<td>14-20</td>
</tr>
</tbody>
</table>

Where \( f_{p-relax} \) is the PISO pressure underrelaxation factor, \( n_{steps} \) is the number of time-steps from which the values are taken, NSP is the number of pressure sweeps and NPCOR is the number of PISO corrector stages. The NSP and NPCOR are given as ranges within which the values of the time steps fall. The optimal pressure relaxation factor is 0.3

Where \( \rho_p \) is the particle density, \( \vec{u}_f \) is the fluid velocity, \( \vec{u}_d \) is the dispersed phase velocity, \( d_p \) is the particle diameter and the key variable for tuning the model is the surface tension \( \sigma \). Weakness of this model is that for hard spheres, such as glass beads, no value of the surface tension is able to force collision over coalescence, without forcing at the same time separation over collision. It is unclear from the Star-CD methodology what happens in case of separation. Transient simulations without solving the temperature-field show that in the cases studied separation means that nothing happens.

No further study of O'Rourke's collision model has been performed, because no transient 2-phase Lagrangian thermally active flow simulation could reach near 900 ms\(^7\).

With the 90°(2 x 2) and the 90° x 120°(10 x 10) meshes a multitude of transient simulations are performed. With the other meshes created, transient simulations are usually only tried once. All resulted in non-convergence after a number of time steps.

The Courant number, defined as \( C_0 = \frac{v \Delta t}{l_{cell}} \), produces values a factor 10 lower than the values reported by Star-CD. Star-CD support e-mailed that this is due to the inclusion of diffusion in their Courant number, while the defined Courant number is based on convection alone. To keep the computed Courant number under 1 a safe time-step in the order of 0.1 ms.

For transient analysis Star-CD only allows use of the PISO algorithm. With the 90°(2 x 2) mesh simulations were performed with a range of values for the PISO pressure underrelaxation, resulting in an optimum at 0.3. See table 6.8.

The simulations with the 90°(2 x 2) mesh are performed starting from the values given in table 6.9 and changing one feature for every next simulation. Subsequently the differencing scheme is changed for all variables from Central Differencing (CD) to Upwind (UD), for \( u_x, u_y, u_z \) and T from UD to QUICK, the time-step size is changed.

\(^7\) The meshes under consideration were 60 cm long and the superficial velocity 2 m/s, which leads to \( 3\tau = 900 \text{ ms} \), where \( \tau \) is the space time.

\(^8\) Where \( v \) is the parcel velocity, \( \Delta t \) is the Lagrangian time-step and \( l_{cell} \) is the body diagonal of the cell.
Table 6.9: Starting values for the $90^\circ(2 \times 2)$ simulation series

<table>
<thead>
<tr>
<th>Time scheme</th>
<th>implicit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time step</td>
<td>0.5 ms</td>
</tr>
<tr>
<td>$\alpha_d$</td>
<td>$4.2 \cdot 10^{-3}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$u_x$</th>
<th>$u_y$</th>
<th>$u_z$</th>
<th>$p$</th>
<th>$k$</th>
<th>$\epsilon$</th>
<th>$T$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10^2</td>
<td>10^2</td>
<td>10^2</td>
<td>10^4</td>
<td>10^2</td>
<td>10^2</td>
<td>10^2</td>
</tr>
<tr>
<td>$f_{\text{relax}}$</td>
<td>0.7</td>
<td>0.7</td>
<td>0.7</td>
<td>0.3</td>
<td>0.7</td>
<td>0.95</td>
</tr>
<tr>
<td>Scheme</td>
<td>CD</td>
<td>CD</td>
<td>CD</td>
<td>CD</td>
<td>CD</td>
<td>CD</td>
</tr>
<tr>
<td>Res.Tol.</td>
<td>$10^{-2}$</td>
<td>$10^{-2}$</td>
<td>$10^{-2}$</td>
<td>$10^{-3}$</td>
<td>$10^{-1}$</td>
<td>$10^{-1}$</td>
</tr>
</tbody>
</table>

Sweeps is the maximum number of sweeps of a variable within a time step, Scheme is the differencing scheme used for the variable, $f_{\text{relax}}$ stands for the relaxation factors, Res.Tol. stands for the residual tolerance of each corrector stage and $\alpha_d$ is the dispersed phase volume fraction, where $\alpha_d = 4.2 \cdot 10^{-3}$ equals 1 weight percent.

from 0.5 ms to 0.3 ms, the differencing schemes of $u_x$, $u_y$, $u_z$ and $T$ from QUICK to MARS, the residual tolerance of $k$, $\epsilon$ and $T$ is changed from $10^{-1}$ to $10^{-2}$ and the relaxation factor for $T$ is changed from 0.95 to 0.7. All simulations fail to converge continuity after 20 to 62 time-steps due to the reaching of the maximum number of PISO corrector stages (NPCOR). When the maximum NPCOR is increased tenfold the same error message occurred in the same time step. The reason for this is the number of $T$ sweeps, which is identical to NPCOR. The explanation is that Star-CD’s thermal energy equation is dependent on all other variables, except pressure for constant density flow and includes multiple second order derivatives. The large number of pressure sweeps, needed for continuity due to the presence of parcels, makes the thermal energy equation even more unstable.

Changing the temporal differencing scheme from implicit to Crank-Nicholson (C.-N.) with a blend factor of $1^{10}$, gets rid of the continuity non-convergence, but introduces error messages of negative values for $k$ and $\epsilon$. Changing the blend factor to 0.5 gives the non-convergence of continuity message. Changing to 0.7 and 0.875 gives a blend of errors, no intermediate error-free blend factor is found.

The simulations performed with the $90^\circ \times 120^\circ(10 \times 10)$ mesh used the same settings as the C.-N. with blend factor 1 of the $90^\circ(2 \times 2)$ simulation with the following deviations: $\alpha_d = 0.01$, the time step is 1 ms and the user-code VISMOLF is activated. Activating VISMOLF couples the molecular viscosity to the temperature. Simulating with blend factors 1, 0.75 and 0.5 resulted in the same error messages as before and a new one: 'Unnormalized residual cannot be reduced to $10^{-10}$ in the pressure correction equation. Round off error rescue not attempted. Solution returned without update.' Blend factor 0.75 even caused a divergence. Reducing the time step size to 0.1 ms gave the new error message only. Implicit simulations

---

9 The T-field is swept once during a corrector stage.
10 Star-CD allows blending of C.-N. and implicit temporal differencing schemes. A blend factor of 1 is full C.-N.
Figure 6.20: Velocity magnitude contour plot of the steady-state simulation in the 90° x 120° (10 x 10) mesh with \( v_{\text{inlet}} = 2.78 \) m/s and \( Pr_t = 0.9 \). The contour plot of the velocity magnitude field is identical to the axial component of velocity. Before the mixing point the velocity profiles are fully developed, after the maximum velocity is lower due to the bigger cross-section resulted in non-convergence of continuity.

The same errors persist for a variety of control variables for two different meshes, thus Star-CD cannot do a transient Lagrangian 2-phase thermally active simulation. Star-CD support acknowledged the problem and e-mailed further that a request for SIMPLE transient analysis was being processed, but would take considerable time before being implemented.

6.5.2 One-phase flow temperature profiles

The simulations are performed in the 90° x 120° (10 x 10) mesh, with an inlet velocity of \( v_{\text{in}} = 2.78 \) m/s in the axial direction, an inlet temperature \( T_{\text{hot}} = 48.0°C \) in the annular region and an inlet temperature \( T_{\text{cold}} = 11.4°C \) in the inlet pipe. In figure 6.20 a contour plot of the velocity magnitude field for this flow is presented. The temperature field values are imported into Fieldview, where the T-profiles of the radial positions at 0.0, 2.8, 6.31 and 7.01 mm are generated. First the effect of the turbulent Prandtl number on the profiles will be treated, after that the effect of a
cross-shaped obstruction.

**Effect of the turbulent Prandtl number**

The turbulent Prandtl number $Pr_t$ is defined in equation 2.32 and appears in the thermal energy equation as summarized in table 2.2. Standard value of $Pr_t$ is 0.9, halving this value would double the thermal energy turbulent diffusion term, causing the thermal energy to mix faster. Figure 6.21 shows three graphs of the experimental values of figure 6.6 together with the simulation results with $Pr_t$ values of respectively 0.9, 0.5 and 0.3. Based on these graphs a Prandtl number of 0.4 would generate results closest to the experimental values.

Keeping the well established Prandtl number at 0.9 this implies that the turbulent viscosity field should be twice as high, which implies that the simulated turbulence is much lower than the experimental values imply. Main source of turbulence is due to strain (see equations 2.37 and 2.30). If the inlet velocities would not be identical this would result in considerable strain at the mixing point. Noticing that $v_{in} = 2.78 \text{ m/s}$ is an average over the time of the entire experiment, this does not necessarily mean that the time averaged inlet-velocities at smaller time scales are identical. Inequalities in the inlet velocities lead to strain, which leads to turbulent energy production\textsuperscript{11}. This would explain the very low $Pr_t$. The importance of knowing the inlet velocities and the possible change in time should not be underestimated.

Another point is the deviation of the starting temperatures of the radial positions 0.0 mm and 2.8 mm. Since the final mean temperature is the same for both simulation and experiment its explanation cannot be that $T_{cold}$ should be about 3°C higher, without changing $T_{hot}$ too. Together with the untypical T-profile at 6.31 mm these would imply a very rapid initial mixing mainly in the center of the pipe. No explanation for this center located mixing can be given. The effect of the cross-shaped measuring device on the mixing will be studied in the next paragraph.

**Effect of a cross-shaped obstruction**

Selection and deletion of a number of cells using the Star-CD 'zone' command, created a one-fourth-of-a-cross shaped gap in the mesh, which surface Star-CD treats as walls. See figure 6.22 for two screen shots. The obstruction blocks 29.5 % of the cross-sectional area, while Signorino's cross blocks a bit more than 19.6 %. Another difference is that the obstruction in the mesh has a smooth surface, while the cross does not, due to the protruding thermocouples. The main reason is the current state of the mesh, which doesn’t allow other gaps. The results will therefore only be treated qualitatively.

Simulating with $Pr_t = 0.9$ the turbulence in front of the obstruction shows no increase, that could explain the increased mixing. Figure 6.23b is a screen-shot of the k-field around the obstruction. However the T-field in figure 6.23a does show a change. This can be explained by the fact that all the water has to pass through the

---

\textsuperscript{11}The sought after k-spot of section 6.3.3:High turbulence area at the mixing zone, which only appears with the oscillations stabilizing QUICK scheme.
Figure 6.21: Simulation results of the $90^\circ \times 120^\circ (10 \times 10)$ mesh with $Pr_t$ at respectively 0.9, 0.5 and 0.3 together with the experimental results. $v_{inlet} = 2.78$ m/s. $T_{cold} = 11.4^\circ$C. $T_{hot} = 48.0^\circ$C.
6.5. SIMULATION OF SIGNORINO’S RESULTS: T

Figure 6.22: Fourth of a cross-shaped obstruction in the mesh.

gap and the cold center stream has to move to the wall, resulting in a temperature drop at all radial positions except the center. See figure 6.24 for the T-profiles at the standard radial positions for the obstructed and the normal flow. If the experimental values are sampled from a T-field with temperature profiles such as figure 6.24a, then the profiles constructed from these samples do not represent the T-field without obstruction.

The effect of the measuring device is quite obvious from the fact that no measurements can be made closer than 2 cm to the mixing point. Whether the disturbance of the cross generates too much turbulence giving rise to too rapid mixing or non-steady values is unknown to me.

It is not possible to simulate the experimental one-phase flow results quantitatively. Reasons for this are

- that the inlet-velocities are not known on a smaller time basis than the total experimental time,

- that the average temperature is well predicted, but the inlet temperatures are not known at the inlet of the pipe, only at some place in the barrels, possibly even only at the heating device display.

- that the effect of the cross is present, but cannot be accounted for without velocity data of the flow around the cross.

Given these results and the impossibility of dilute and dense two-phase flow analysis further experimentation with different volume fractions of the dispersed phase seems premature. First the flow has to be thoroughly assessed by measurements on the places indicated.
CHAPTER 6. SIMULATION RESULTS AND DISCUSSION

(a) Contour plot of the T-field. Clear distortion of the field in front of the obstruction.

(b) Contour plot of the k-field. Zoom in around the obstruction. No significant increase in turbulence before the obstruction. Directly after there is a high turbulence spot.

Figure 6.23: Effect of the obstruction on T and k fields.

6.6 Volume Fraction Field Dependence on the Transverse Lift Force

With only steady-state analysis possible and non-rotating particles\textsuperscript{12} the only standard force not taken into account by Star-CD is the transverse lift force. First the implementation of Sommerfeld's formulation [12] of the transverse lift force in Star-CD is treated in the introduction, after which the results of very dilute two-phase flow simulation in channel and pipe are presented.

6.6.1 Introduction

Star-CD only allows implementation of body forces using the user-code DROMOM.F (See appendix E.2). These forces are not taken as interaction forces between the continuous and the dispersed phase and do not contribute directly to the momentum source terms of the continuous momentum equations. This restricts the use to one-way coupling, that is to volume fractions below $\alpha_d = 10^{-6}$. This restriction is removed, when the momentum source terms are programmed by user-coding based on trajectory information.

The calculation of the transverse lift force follows Sommerfeld's [12] or Laín's [11] formulation and uses the values of the cell averaged velocity-component gradients. Because the values of these variables are again not available in the user-coded subroutine, the following strategy is used. First nine scalars are defined in pro-star, the pre-/post-processing program of Star-CD. They are set up as 'passive' and the solver is set to 'user', thereby enabling the user-code SCALFN.F, (see appendix E.3,) with which the nine velocity-component gradients are assigned to the nine scalars. These scalars are available in the DROMOM.F.

\textsuperscript{12}See chapter 3, thereby the accelerated or added mass force, the history-force and the Magnus-force are excluded. For an explanation of the these forces see Sommerfeld [12] or [7].
6.6. VOLUME FRACTION FIELD DEPENDENCE ON THE TRANSVERSE LIFT FORCE

Figure 6.24: Effect of the obstruction on the T-profiles. From top to bottom the profiles are at the radial positions of respectively 7.01 mm, 6.31 mm, 2.8 mm and 0.0 mm. The place of the obstruction is visible in the graph as the gap in the two lower profiles. The dots mark the temperatures at the position of the thermocouples. Profiles made by plotting the dotted temperatures for various positions of the obstruction, do not represent the non-obstructed flow. Temperature in °C, distance from the mixing-point in cm.
6.6.2 Effect of Transverse Lift Force for Stojanovic’s Channel-flow

The motion of parcels though the channel is determined by initial position and velocity, acting forces and whether the turbulent dispersion is switched on. The parcels start at their respective positions with 90% of the fluid velocity in the axial direction. The acting forces are the pressure force, the gravity force and drag force (without the turbulent dispersion). All forces are aligned to the axial direction, resulting in straight trajectories. See figure 6.25a and b. Activating the turbulent dispersion the parcels get a random kick from the fluid resulting in the trajectories of figure 6.25c and d. The parcels are pseudo-randomly\(^{13}\) initialized at \(z=0\) limited to the area 1 mm off the walls. During the flow through the channel the dispersed phase volume fraction distribution becomes more ordered. A lower volume fraction at the wall, followed by a higher fraction at about 1.5 cm off the wall of about 0.9 cm thick. The explanation for the higher fraction is the wall-parcel interaction. The parcels get a random radial velocity due to the turbulent dispersion. Those that hit the wall, bounce off the wall. Due to drag the radial velocity is reduced to zero, causing an increase of parcels present in the higher volume fraction area. See figure 6.26 for contour plots. Contour plots of volume fraction fields are identical for inlet volume fractions of \(0.01\) and \(10^{-6}\) due to the scaling of the contours. Since the parcels do not interact and the number of parcels used was identical, this is as expected since Star-CD’s momentum coupling is not sufficient for two-way coupling. This is a confirmation of the simulation results of section 6.4.

A simulation with the transverse lift force turned on by activating DROMOM.F, gives an identical volume fraction field. No effect of the transverse lift force on the field is present.

The transverse lift force points in the direction of the higher velocity, that is in the direction of the center of the channel. As such it promotes order in the volume fraction field: higher volume fractions toward the center. The turbulent dispersion creates disorder. The explanation for the lack of effect of the transverse lift force on the field is that the turbulent dispersion, that is the drag force \((F_D \sim d_p^2)\) on a 100 \(\mu m\) particle is much stronger in this air/particle flow than the transverse lift force \((F_H \sim d_p^3)\).

6.6.3 Effect of Transverse Lift Force for Flow in Pipe

The parcels are initialized with 100% of the continuous phase velocity. The same results are found as in the channel flow:

- Inlet volume fractions of \(0.01\), \(10^{-4}\) and \(10^{-6}\) give qualitatively identical contour plots of the \(\alpha_d\)-fields.

- No effect of the transverse lift force on the volume fraction field.

\(^{13}\)Using the Star-CD Fortran SRAND(SEED) and RAND() functions to generate a lot of initial positions. See figure 6.26a for the resulting average \(\alpha_d\)-distribution.
(a) Active forces are $F_D$, $F_g$ and $F_p$. No dispersion. Visualization of parcels with velocity vectors.

(b) Zoom of (a). Mainly big velocity vectors with small parcel dots.

(c) Active forces are $F_D$, $F_g$ and $F_p$. Dispersion active. Visualization of parcels with velocity vectors.

(d) Zoom of (c).

Figure 6.25: Four screen-shots of selected parcel tracks of a steady-state simulation in the channel mesh with an inlet dispersed phase volume fraction $\alpha_d = 10^{-6}$. Sub-figures (a) and (b) are without turbulent dispersion, while (c) and (d) are with turbulent dispersion. The length of the velocity vectors in the upper two figures are different from the lower figures due to the different perspective of the screen-shots.
Figure 6.26: Two screen-shots of cross-sections of the dispersed phase volume fraction field in channel mesh. The cross-section are taken at the inlet and the outlet of the channel.
6.6. VOLUME FRACTION FIELD DEPENDENCE ON THE TRANSVERSE LIFT FORCE

Figure 6.27: Two screen-shots of the volume fraction field of the water/particle flow through the pipe mesh. Inlet volume fraction is $\alpha_d = 10^{-6}$.

The volume fraction field has a small volume fraction build-up at the wall\textsuperscript{14}. The highest volume fraction zone at the wall is on one side of the pipe only for all three volume fractions. Their is no explanation for this on basis of the models. It has to be accounted for as a numerical error in Star-CD’s Lagrangian analysis. See figure 6.27.

\textsuperscript{14}This is absent in the air/particle flow due to the low viscosity of air and hence of the chance of a parcel to get stuck in the laminar flow.
Chapter 7

Conclusion and Recommendations

- Mesh creation in Star-CD for two-phase flow faces the problems of minimum cell volume and of center and wall accumulation of the dispersed phase. Any mesh creation in Star-CD has the problem of coupling non-uniformly shaped cells.

- Star-CD is capable of simulating one-phase grid generated turbulence decay.

- It is possible to qualitatively simulate one-phase turbulent pipe mixing of water streams differing in temperature. Quantitatively correct simulations could not be performed, due to the lack of information about the inlet variables and about the effect of the measuring device used.

- Turbulent two-phase flow has different mixing characteristics than one-phase flow. This is well established in literature for pipe flow and jet flow. The focus in this project was on the experimental results due to Signorino. The different mixing characteristics can be attributed to the change in $k$ and $\epsilon$ due to the presence of particles: turbulence modulation.

- Star-CD is not able to generate realistic two-phase simulation results, due to its inability to handle the effect of particle presence on $k$ and $\epsilon$. Implementation of this effect in their respective equations through user-code is as yet not possible. This is due to the file handling of the Star-CD version 3.15 code, which prohibits the access to the trajectory information from which source terms for the momentum, thermal energy, $k$ and $\epsilon$ equations can be calculated.

- Star-CD is not able to simulate transient thermally active two-phase flow.

- The implementation of the transverse lift force has no impact on the dispersed phase distribution in very dilute flow for both the channel and the pipe mesh. For the steady-state analysis of very dilute flow the forces implemented by Star-CD, i.e. drag, pressure and gravity force are sufficient.
Other codes are designed and working for two-phase flow. For example is LAG3D a code for parcel tracking and coupling terms calculation, designed by Sommerfeld. In combination with a finite volume code such as FASTEST Stojanovic has been able to do two-phase calculations. Star-CD cannot be said to be up to the job! I recommend using a working code.
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Appendix A

Derivation of the k-equation

For the derivation of the k equation the manipulations of the Navier-Stokes equation as suggested in 2.34 are done. First the difference of the Navier-Stokes equation (2.13) and the RANS equations (2.23) is taken, giving the equation of change of the fluctuating velocity-component:

\[
\frac{\partial u_i}{\partial t} - \frac{\partial \bar{u}_i}{\partial t} = \frac{\partial u'_i}{\partial t} = -u_j \cdot \frac{\partial u'_i}{\partial x_j} - \frac{1}{\rho} \frac{\partial p'}{\partial x_i} + \nu \cdot \frac{\partial^2 (u'_i)}{\partial x_j \partial x_j} + \frac{\partial u'_j \cdot u'_i}{\partial x_j} - u'_j \cdot \frac{\partial \bar{u}_i}{\partial x_j}
\]

On the right-hand side the first three terms are the fluctuating counterparts of the three terms in the Navier-Stokes equation, the fourth is the gradient in the Reynolds stresses and the new term is the turbulent transport of the average momentum. The product of \(u'_i\) and \(\frac{\partial \bar{u}_i}{\partial t}\) is averaged, resulting in an equation for the change of k:

\[
\frac{\partial k}{\partial t} = -u'_j \cdot u_j \frac{\partial u'_i}{\partial x_j} - \frac{u'_k}{\rho} \frac{\partial p'}{\partial x_i} + u'_j \frac{\partial^2 u'_i}{\partial x_j \partial x_j} + u'_i \frac{\partial u'_j \cdot u'_i}{\partial x_j} - u'_j \cdot \frac{\partial \bar{u}_i}{\partial x_j}
\]

The five terms in this equation will be worked out separately, after which the k equation will be recomposed.

A:

\[
\begin{align*}
u'_i \cdot u_j \cdot \frac{\partial u'_i}{\partial x_j} &= \nu'_i \cdot (\bar{u}_j + u'_j) \cdot \frac{\partial u'_i}{\partial x_j} = \bar{u}_j \cdot \frac{\partial}{\partial x_j} \left( \frac{1}{2} u'_i \cdot u'_i \right) + \\
u'_j \cdot \frac{\partial}{\partial x_j} \left( \frac{1}{2} u'_i \cdot u'_i \right) &= \bar{u}_j \cdot \frac{\partial}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \frac{1}{2} u'_i \cdot u'_i \cdot u'_j \right) + \\
-\frac{1}{2} u'_i \cdot u'_i \cdot \frac{\partial u'_j}{\partial x_j} &= \bar{u}_j \cdot \frac{\partial}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \frac{1}{2} u'_i \cdot u'_i \cdot u'_j \right)
\end{align*}
\]

eq. 2.9=0
APPENDIX A. DERIVATION OF THE K-EQUATION

Term A results in a convective transport term for k and a third order correlation representing the turbulent k flux.

\[ \frac{u'_i}{\rho} \cdot \frac{\partial \rho'}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \frac{\rho'}{\rho} \cdot u'_i \frac{\partial u'_i}{\partial x_i} \right) - \frac{\rho'}{\rho} \cdot \frac{\partial u'_i}{\partial x_i} \]

eq. 2.9 = 0

Term B represents the pressure diffusion of k.

\[ \nu \cdot \frac{\partial u'_i}{\partial x_j \partial x_j} = \nu \frac{\partial}{\partial x_j} \left( u'_i \cdot \frac{\partial u'_i}{\partial x_j} \right) - \nu \frac{\partial u'_i}{\partial x_j} \frac{\partial u'_i}{\partial x_j} = \nu \frac{\partial}{\partial x_j} \left( u'_i \cdot \frac{\partial u'_i}{\partial x_j} \right) + \]

\[ + \nu \frac{\partial u'_i}{\partial x_j} \cdot \frac{\partial u'_j}{\partial x_j} - \nu \left( \frac{1}{2} \frac{\partial u'_i}{\partial x_j} + \frac{1}{2} \frac{\partial u'_j}{\partial x_i} + \frac{\partial u'_i}{\partial x_j} \cdot \frac{\partial u'_j}{\partial x_i} \right) = \]

\[ \nu \frac{\partial}{\partial x_j} \left( u'_i \cdot \frac{\partial u'_i}{\partial x_j} \right) + \nu \frac{\partial}{\partial x_j} \left( u'_i \cdot \frac{\partial u'_j}{\partial x_i} \right) - \nu \cdot u'_i \cdot \frac{\partial}{\partial x_j} \left( \frac{\partial u'_i}{\partial x_j} \right) + \]

eq. 2.9 = 0

\[ -2\nu \cdot s'_{ij} \cdot s'_{ij} = \frac{\partial}{\partial x_j} \left( 2\nu \cdot u'_i \cdot s'_{ij} \right) - \epsilon \]

Term C results in the turbulent kinetic energy dissipation \( \epsilon \) and a term representing the viscous diffusion of k.

Term D vanishes by definition.

\[ u'_i \cdot \frac{\partial u'_j}{\partial x_j} = u'_i \cdot \frac{\partial u'_j}{\partial x_j} = 0 \]

Term D vanishes by definition.

Term E is always positive and represents the turbulent kinetic energy production P. Rearranging gives the k-equation, which is identical to equation 5.132 of Pope [4]:

\[ \frac{\partial k}{\partial t} = -u'_j \cdot \frac{\partial u'_i}{\partial x_j} - \frac{\partial}{\partial x_j} T_j + P - \epsilon \]

where

\[ T_j = \frac{1}{2} \cdot u'_i \cdot u'_i + \frac{\rho'}{\rho} \cdot \frac{\partial u'_i}{\partial x_j} - 2\nu \cdot u'_i \cdot s'_{ij} \]
Appendix B

Derivation of Modeled Average Fluctuation Products

The modeling of the turbulent kinetic energy production term \( P \) (2.37) and the gradients in the Reynolds stresses and in the turbulent thermal energy fluxes with the Boussinesque assumption (2.28) and analogon (2.32) leads to the following terms for incompressible fluid flow:

\[
\begin{align*}
\frac{\partial u_i' u_j'}{\partial x_j} &= \frac{\partial}{\partial x_j} \left( -2 \nu_i \bar{s}_{ij} + \frac{2}{3} k \delta_{ij} \right) = \\
&= \frac{\partial}{\partial x_j} \left( \nu_i \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right) + \frac{\partial}{\partial x_j} \left( \frac{1}{3} u_i' u_j' \delta_{ij} \right) \\
A &= \frac{1}{3} \frac{\partial u_i' u_j'}{\partial x_i} = \frac{1}{3} \nu \frac{\partial u_i'}{\partial x_i} = 0 \\
B &= - \frac{\partial}{\partial x_j} \left( \nu_i \left( \frac{\partial u_i}{\partial x_j} \right) \right) - \frac{\partial}{\partial x_j} \left( \nu_i \frac{\partial u_j}{\partial x_i} \right) \\
C &= - \frac{\partial \nu_i \partial u_j}{\partial x_i \partial x_j} - \nu_i \frac{\partial^2 u_j}{\partial x_i \partial x_j} - \nu_i \frac{\partial}{\partial x_i} \left( \frac{\partial u_j}{\partial x_j} \right) = 0
\end{align*}
\]

thus:

\[
\begin{align*}
\frac{\partial u_i' u_j'}{\partial x_j} &= - \frac{\partial}{\partial x_j} \left( \nu_i \left( \frac{\partial u_i}{\partial x_j} \right) \right) \quad (B.1) \\
\text{and} \quad \frac{\partial c_p T' u_j'}{\partial x_i} &= - \frac{\partial}{\partial x_i} \left( \frac{c_p T}{P_{rt}} \frac{\partial u_j}{\partial x_i} \right) \quad (B.2) \\
\text{and} \quad P &= -u_i' u_j' \frac{\partial u_i}{\partial x_j} = 2 \nu_i \bar{s}_{ij} \frac{\partial u_i}{\partial x_j} - \frac{2}{3} k \delta_{ij} \frac{\partial u_i}{\partial x_j} \\
D &= \frac{2}{3} k \delta_{ij} \frac{\partial u_i}{\partial x_j} \quad \text{E}
\end{align*}
\]
APPENDIX B. DERIVATION OF MODELED AVERAGE FLUCTUATION PRODUCTS

\[ D = \nu_t \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \frac{\partial u_i}{\partial x_i} = \nu_t \left( \frac{\partial u_i}{\partial x_i} \frac{\partial u_j}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \frac{\partial u_i}{\partial x_j} \right) = \nu_t \frac{\partial \bar{u}_i}{\partial x_i} \frac{\partial \bar{u}_j}{\partial x_j} + \nu_t \frac{\partial \bar{u}_j}{\partial x_i} \frac{\partial \bar{u}_i}{\partial x_j} \]

\[ E = \frac{2}{3} k \frac{\partial \bar{u}_i}{\partial x_i} = 0 \]

thus \[ P = \nu_t \frac{\partial \bar{u}_j}{\partial x_i} \frac{\partial \bar{u}_i}{\partial x_j} \] (B.3)
Appendix C

Comparisons between Continuous Phase equations

C.1 Gouesbet and Star-CD

Comparison is made on basis of the general equation:

$$\frac{\partial}{\partial x_j}(\rho u_j \phi) = \frac{\partial}{\partial x_j}(\Gamma \frac{\partial \phi}{\partial x_j}) + S_\phi + S_{\phi p}$$

Differences:

- Gouesbet does not take into account the thermal energy production due to turbulent energy dissipation.

- Gouesbet does not use an effective density $\alpha_c \rho_c$ or viscosity like Star-CD. This use is typical for Euler-Lagrange approach, placing Star-CD in an in between region between Euler-Euler and Euler-Lagrange analysis. Star-CD states that the volume fraction is taken into account to allow simulation with a higher loading of the particulate phase.

- Gouesbet does not subtract the effect of the pressure force from the change of momentum of the particle, to account for the interaction between the phases.

C.2 Crowe and Star-CD

Comparison is made on basis of the general equation:

$$\frac{\partial}{\partial t}(\rho \phi) + \frac{\partial}{\partial x_j}(\rho u_j \phi) = \frac{\partial}{\partial x_j}(\Gamma \frac{\partial \phi}{\partial x_j}) + S_\phi + S_{\phi p}$$

Differences:

- Crowe does not subtract the gravity acceleration form the $\overline{S_{u \rho p}}$. 
Table C.1: Comparison of cont. phase equations of Gouesbet and Star-CD

<table>
<thead>
<tr>
<th>$\phi$</th>
<th>$\Gamma$</th>
<th>$S_\phi$</th>
<th>$S_{\phi P}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u_{i, \text{star}}$</td>
<td>$\alpha_c (\mu + \mu_t)$</td>
<td>$-\alpha_c \frac{\partial}{\partial x_i} (p + \frac{3}{2} \rho_c k)$</td>
<td>$-\frac{1}{n_d} \sum_{\n_d} \sum_{\n_d} \left( \frac{v_{\text{new}} - v_{\text{old}}}{d_{\text{Lag}}} \right)$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$u_{i, \text{Goues}}$</td>
<td>$\mu + \mu_t$</td>
<td>$-\frac{\partial}{\partial x_i} (p + \frac{3}{2} \rho_c k)$</td>
<td>$-n \left( m_p \left( \frac{dv_i}{dt} - g_i \right) \right)$</td>
</tr>
<tr>
<td>$k_{\text{star}}$</td>
<td>$\alpha_c (\mu + \mu_t)$</td>
<td>$\alpha_c \frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j}$</td>
<td>$-\rho \epsilon$</td>
</tr>
<tr>
<td>$k_{\text{Goues}}$</td>
<td>$\frac{\mu_c}{\sigma_c}$</td>
<td>$\frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j} + c_c \rho_c \epsilon$</td>
<td>$S_{k_{\text{Goues}}} \rightarrow \text{user-code}$</td>
</tr>
<tr>
<td>$\epsilon_{\text{star}}$</td>
<td>$\alpha_c (\mu + \mu_t)$</td>
<td>$\epsilon \left( C_{1.5} \alpha_c \frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j} + \right.$</td>
<td>$S_{\epsilon_{\text{star}}} \rightarrow \text{user-code}$</td>
</tr>
<tr>
<td></td>
<td>$\sigma_c$</td>
<td>$\left. - C_{2.5} \rho_c \epsilon \right)$</td>
<td>$C_{c3.5} \epsilon S_{k_{\text{Goues}}}$</td>
</tr>
<tr>
<td>$\epsilon_{\text{Goues}}$</td>
<td>$\frac{\mu_c}{\sigma_c}$</td>
<td>$\epsilon \left( C_{1.5} \frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j} + \right.$</td>
<td>$\epsilon_{\text{Goues}}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\left. - C_{2.5} \rho_c \epsilon \right)$</td>
<td>$C_{c3.5} \epsilon S_{k_{\text{Goues}}}$</td>
</tr>
<tr>
<td>$c_v T_{\text{star}}$</td>
<td>$\alpha_c \left( \frac{\mu}{P_r} + \frac{\mu_t}{P_{r_t}} \right)$</td>
<td>$\alpha_c (\mu + \mu_t) \frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j}$</td>
<td>$-\frac{1}{n_d} \sum_{\n_d} \sum_{\n_d} \left( \frac{c_{v_{\text{new}}} (T_{\text{new}} - T_{\text{old}})}{d_{\text{Lag}}} \right)$</td>
</tr>
<tr>
<td>$c_v T_{\text{Goues}}$</td>
<td>$\frac{\mu}{P_r} + \frac{\mu_t}{P_{r_t}}$</td>
<td>$\left( \frac{\mu}{P_r} + \frac{\mu_t}{P_{r_t}} \right)$</td>
<td>$-n \left( 4 \pi r^2 g \right)$</td>
</tr>
</tbody>
</table>

Where $\alpha_c$ is the continuous phase volume fraction, $\rho_c$ is the continuous phase fluid density, $\mu$ is the continuous phase molecular viscosity, $\rho_o$ is a reference density, $\sum_d$ stands for summation over all dispersed phase parcels, $n_p$ is the number of Lagrangian time steps the parcel needed to traverse the cell, $d_{\text{Lag}}$ is the Lagrangian time step, $v_{\text{new}}$ and $v_{\text{old}}$ are respectively the new and the old value of the velocity-component of a parcel in the trajectory, $n$ is the average number of particles in a cell, $\langle \rangle$ stands for volume-averaging and $c_D$ is an undefined parameter, probably for tuning. The other variables and constants are as defined in the previous chapters. Gouesbet uses $\rho_c$ for $\rho$, while Star-CD uses $\alpha_c \rho_c$ for $\rho$. 
Crowe has the turbulent energy dissipation as $\alpha_c \epsilon$, defined as $\epsilon \equiv \mu_c \frac{\partial u'_i}{\partial x_j} \frac{\partial u'_j}{\partial x_i}$ instead of solving a balance equation of $\epsilon$. Crowe presupposes DNS.

Important in this comparison is the fact that Crowe’s Eulerian approach also uses $\alpha_c$ in the same way as Star-CD.

### Table C.2: Comparison of continuous phase equations of Crowe and Star-CD

<table>
<thead>
<tr>
<th>$\phi$</th>
<th>$\Gamma$</th>
<th>$S_\phi$</th>
<th>$S_{\phi p}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u_{i, \text{star}}$</td>
<td>$\alpha_c \mu$</td>
<td>$- \frac{\partial}{\partial x_j} (\alpha_c \rho_i c u'<em>i u'<em>j) - \frac{\partial \rho}{\partial x_j} + \frac{1}{n_d} \sum</em>{p} \sum</em>{m_d} \left( m_d v^n_i - v^n_j \right) + g_i (\rho - \alpha_c \rho_o) - F_{g,i} - F_{p,i}$</td>
<td>$-F_{g,i} - F_{p,i}$</td>
</tr>
<tr>
<td>$u_{i, \text{Crowe}}$</td>
<td>$\alpha_c \rho_o$</td>
<td>$\alpha_c \rho_o c u'<em>i u'<em>j = \alpha_c \rho_o \frac{\partial \rho}{\partial x_j} + \frac{1}{n_d} \sum</em>{p} \sum</em>{m_d} \left( m_d v^n_i - v^n_j \right)$</td>
<td>$-\beta_v (u_i - \bar{v}_i)$</td>
</tr>
<tr>
<td>$k_{\text{star}}$</td>
<td>$\frac{\alpha_c (\mu + \mu_o)}{\sigma_k}$</td>
<td>$- \alpha_c \rho_o c u'_i u'_j \frac{\partial u_i}{\partial x_j} - \rho \epsilon$</td>
<td>$S_{kp}$</td>
</tr>
<tr>
<td>$k_{\text{Crowe}}$</td>
<td>$\frac{\sigma_k}{\mu_c}$</td>
<td>$- \rho \frac{\partial u'_i}{\partial x_j} \frac{\partial u'_j}{\partial x_i} - \alpha_c \epsilon$</td>
<td>$\beta_v (</td>
</tr>
</tbody>
</table>

Where $\rho$ is $\alpha_c \rho_o$, $\alpha_c$ is the continuous phase volume fraction, $\rho_c$ is the continuous phase fluid density, $\mu$ is the continuous phase molecular viscosity, $\rho_o$ is a reference density, $\sum_{m_d}$ stands for summation over all dispersed phase parcels, $n_p$ is the number of Lagrangian time step the parcel needed to traverse the cell, $\delta t$ is the Lagrangian time step, $\beta_v$ is Crowe’s constant, which contains all terms necessary to formulate the drag-force between the phases, $u_i$ is the fluid-phase velocity component and $v_i$ is the velocity component of a parcel.
Appendix D

Input-Files

D.1 Stojanovic’s channel flow simulation

This input-file makes a grid following the publication of Stojanovic and sets up the Star-CD environment for the simulation, which results can be compared with experimental the results.

Defining parameters
lx, ly, lz are the dimensions of the grid in meter.
*set lx 0.2
*set ly 0.2
*set lz 2.0
ncx, ncy, ncz are the number of cells in resp. x, y and z direction.
*set ncx 34
*set ncy 34
*set ncz 74
vin is the mean flow velocity in m/s used for the inflow boundary
*set vin 10

Mesh generation
*set dx lx / ncx
*set dy ly / ncy
*set dz lz / ncz

Boundary definition
*set kin 0.75
*set epsin 100
rdef, 0, wall, standard
nosl, stand, 9, 0, 0, 0, 1, 0
rname, 0, Wall
rinlet, mass, kep5
init, stan, 0, 0, 0, 1, 0, kep5, 0.1, 0.25, 293
rdef, 1, inlet, standard
APPENDIX D. INPUT-FILES

0,0,vin,1,0,kin,epsin,1.205,
name,1,Inlet
rdef,2,outlet,standard
split,1,
name,2,outlet
bread,Stoj.bnd,0,all,,add,code

! Air properties
+set kinit 0.1
+set epsinit 0.25
pmat.l,fluid,AIR
dens,constant,1.205
visc,constant,1.81e-05
spec,constant,1006
cond,constant,0.02637
turb,ke,1,stan
lowre,off
coke,0.09,1.44,1.92,1.44,-0.33,0.419,1.219,0.9,,
pmat.l,fluid
temp,off
accel,0,0,9.81,0.105882,0.1,0.000000,1.205
init,stan,0,0,1,0,0,0,keps,kinit,epsinit,293
moni,84984
pres,1.0e+05,85020
tdatum,273
accel, 0.000000,0.000000, 9.810000, 0.105882,0.100000,0.000000,1.205

! Control parameters
time,steady,nodefa
tphl,off
f surf,off
algor,simple,,,
iter,0.001
solu,scalar
solve,y,y,y,y,y,n,n,n,n,n,
relax,0.7,0.3,0.7, ,1, , , ,
sweep,100,100,100,1000,100,100, ,
resid,0.1,0.1,0.1,0.05,0.1,0.1, ,
dsch,ud,uvu,,stan
dsch,ud,turb,,stan

! Lagrangian Setup. Execute only when simulating 2-phase flow.
tphl,on
f surf,off
tphl,on,uncoupled,0.35
drturbulent,off
draverage,off
drpost,200,100

memo maxdrp 2000
drin,user,2000
drtype,1
drmomentum,standard,0,0
derheat,off,
drbreakup,off,,
drvall,rebound,
dcollision,off
drboil,off
drprop,dens,standard,2440
drprop,etcco,standard,0.02
drprop,cp,user
drprop,hova,standard
D.2. STAR-CD SETUP FOR STOJANOVIC CHANNEL FLOW

D.2 Star-CD setup for Stojanovic channel flow

! This input file defines the Star-CD setup for
! the simulations of Stojanovic's channel flow.

! Boundary definition
*set kin 0.75
*set epsin 100
rdef,0,wall,standard$nosl,stand,9, 0,0,0,1,0
rname,0,Default_Boundary_Region
rdef,0,wall,keps
rname,0,0,0,1,0,0,keps,0,1,0.25,293
rname,1,Inlet
rdef,1,inlet,standard
0,0,vin,1,0,kinit,epsinit,1.205,
rdef,2,outlet,standard
rname,2,Outlet
broad.Stoj.bnd.O.all,,add,code

! Air properties
*set kinit 0.1
*set epsinit 0.25
pmat,1,fluid,AIR
dens,constant,1.205
Ivis,constant,1.81e-05
spec,constant,1006
cond,constant,0.02637
turb,ke,1,stan
tau,off
coke,0.09,1.44,1.92,1.44,-0.33,0.419,1,1.219,0.9,,
pmat,1,fluid
temp,off
accel,0,0,9.81,0.105882,0.100000,0.000000,1.205
cini,y,,0
init,stan,0,0,0,1,0,0,keps,kinit,epsinit,293
moni,84984
pres,1.4e05,85020
tdatum,273
core,0.000000,0.000000,9.810000,0.105882,0.100000,0.000000,1.205

! Control parameters
time,steady,nodefa
tphl,off
fsurf,off
algor,simple,,
iter,0.001
solut,scalar
solve,y,y,y,y,y,y,n,n,n,n,
relax,0.7,0.3,0.7,,1,,
sweep,100,100,100,1000,100,100,,
resid,0.1,0.1,1,0.0,0.1,0.1,,
dsch,ud,uvw,stan
dsch,ud,turb,stan

! Lagrangian Setup
! Execute only when for Lagrangian analysis
D.3 5° and 25° mesh creation input file

```plaintext
# Example input file for mesh creation

# Parameter definition for vertex creation

# Example of parameter values

# Example of mesh specifications

# Example of mesh generation commands
```

APPENDIX D. INPUT FILES
D.3. 5° AND 25° MESH CREATION INPUT-FILE

*set znorm 10e-3
*set rnorm 0.3e-3
*set zn znorm / 2
*set L1 z1 - zn - mzlength
*set L2 z2 - z1 - znorm
*set L3 z3 - z2 - znorm
*set L4 pipelength - z3 - zn

!!! ***********************************************************
!!! Vertex creation !!!
!!! ***********************************************************
csys 1
! V, NV1, X, Y, Z
! Defines a vertex in the currently active local coordinate system.
! NV1 - Vertex number.
! X, Y, Z - Coordinates of point (R, Theta, Z in cylindrical or R,
! Theta, Phi in spherical and toroidal).

! First 16 cm : inlet and mixingzone
v 1 0 0 0
v 2 rmax 0 0
v 3 rmax 0 mzlength
v 4 rmax 0 mzlength
v 5 ri1 0 0
v 6 ri2 0 0
v 7 ri2 0 itlength
v 8 ri2 0 itlength
v 9 rlstcell 0 0
v 10 ri1 - rnorm 0 0
v 11 ri2 + rnorm 0 0
v 12 rmax - rnorm - rnorm 0 0
v 13 0 0 itlength
v 14 rlstcell 0 itlength
v 15 ri1 - rnorm 0 itlength
v 16 ri2 + rnorm 0 itlength
v 17 rmax - rnorm - rnorm 0 itlength
v 18 rmax 0 itlength
v 19 rlstcell 0 mzlength
v 20 ri1 - rnorm 0 mzlength
v 21 ri1 0 mzlength
v 22 ri2 0 mzlength
v 23 ri2 + rnorm 0 mzlength
v 24 rmax - rnorm - rnorm 0 mzlength

! Introducing the needed vertices for the three measurement blocks
v 25 0 0 z1 - zn
v 26 rlstcell 0 z1 - zn
v 27 ri1 - rnorm 0 z1 - zn
v 28 ri1 0 z1 - zn
v 29 ri2 0 z1 - zn
v 30 ri2 + rnorm 0 z1 - zn
v 31 rmax - rnorm - rnorm 0 z1 - zn
v 32 rmax 0 z1 - zn
v 33 0 0 z1 + zn
v 34 rlstcell 0 z1 + zn
v 35 ri1 - rnorm 0 z1 + zn
v 36 ri1 0 z1 + zn
v 37 ri2 0 z1 + zn
v 38 ri2 + rnorm 0 z1 + zn
v 39 rmax - rnorm - rnorm 0 z1 + zn
v 40 rmax 0 z1 + zn
v 41 0 0 z2 - zn
v 42 rlstcell 0 z2 - zn
v 43 ril - rnorm 0 z2 - zn
v 44 ril 0 z2 - zn
v 45 ri2 0 z2 - zn
v 46 ri2 + rnorm 0 z2 - zn
v 47 rmax - rnorm - rnorm 0 z2 - zn
v 48 rmax 0 z2 - zn
v 49 0 0 z2 + zn
v 50 rlstcell 0 z2 + zn
v 51 ril - rnorm 0 z2 + zn
v 52 ril 0 z2 + zn
v 53 ri2 0 z2 + zn
v 54 ri2 + rnorm 0 z2 + zn
v 55 rmax - rnorm - rnorm 0 z2 + zn
v 56 rmax 0 z2 + zn
v 57 0 0 z3 - zn
v 58 rlstcell 0 z3 - zn
v 59 ril - rnorm 0 z3 - zn
v 60 ril 0 z3 - zn
v 61 ri2 0 z3 - zn
v 62 ri2 + rnorm 0 z3 - zn
v 63 rmax - rnorm - rnorm 0 z3 - zn
v 64 rmax 0 z3 - zn
v 65 0 0 z3 + zn
v 66 rlstcell 0 z3 + zn
v 67 ril - rnorm 0 z3 + zn
v 68 ril 0 z3 + zn
v 69 ri2 0 z3 + zn
v 70 ri2 + rnorm 0 z3 + zn
v 71 rmax - rnorm - rnorm 0 z3 + zn
v 72 rmax 0 z3 + zn
v 73 0 0 pipelength
v 74 rlstcell 0 pipelength
v 75 ril - rnorm 0 pipelength
v 76 ril 0 pipelength
v 77 ri2 0 pipelength
v 78 ri2 + rnorm 0 pipelength
v 79 rmax - rnorm - rnorm 0 pipelength
v 80 rmax 0 pipelength

vset all

*set anz1 1
*set anz2 ril - rnorm - rlstcell / rnorm
*set anz3 3
*set anz5 3
*set anz6 rmax - ri2 / rnorm
*set anz7 7
*set anz8 itlength / znorm + 1
*set anz9 mzlength - itlength / znorm + 1

*set ra10 1.0
*set ra11 1.1
*set ra0878 0.95
*set ra08 0.85
D.3. 5° AND 25° MESH CREATION INPUT-FILE

```
! CTABLE, ICTID(I), COPTION, ICOL, IPOR(O), IMAT(I), ISPIN(I), IGROUP(O),
! LIMAT(I), IPROC(O), RADI, THICKCO.), FSHAT
! Defines a cell table entry.
! ICTID - Arbitrary reference ID for this entry. All cells generated
! with this ICTID will have the characteristics associated
! with this entry.
! COPTION - SHELL
! For dummy three-, four-, five-, or six-noded cells. This
! option is useful for some mesh generation functions
! (surface representations), and post-processing functions
! (displays of boundary data), but has no actual bearing
! on any STAR analysis.
! ICOL - Color table index for all cells referenced to this table.
! IPOR - Porous material property reference for all (FLUID) cells
! referenced to this table. Use IPOR = 0 to indicate
! completely free flowing fluid.
! IMAT - Material property (fluid or solid) reference number.
! ISPIN - Spin index used for implicit treatment of multiple
! rotational frames of reference.

ctab 5 shell 6 0 1 1
ctyp 5

! PATCH, NV1, NV2, NV3, NV4, NCI, NCJ, NVINCI, NVINCJ, NVSTART, CREDPT,
! ICSRF(O), NITER(O), TOL(.00001), RLXF(.9), RAT10(1.), RAT10J(1.)
! Creates a (structured) surface bounded by up to four splines. The
! surface consists of vertices and shell cells. Any edge not contained
! in a spline reverts to a straight line between two corners. Edges can
! span entire splines or only parts of them. Any discontinuous
! (negative) vertices on an edge spline will be treated as a fixed
! point. Newly created shells are given the reference number (ICTID) of
! the currently active cell type.

! NV1, ..., NV4 - ID numbers of four corner vertices.
! NCI - Number of cells in the I direction (parallel to NV1-NV2).
! NCJ - Number of cells in the J direction (parallel to NV1-NV4).
! NVINCI, NVINCJ - Increments between adjacent vertices in the I
! and J directions, respectively.
! NVSTART - Vertex number of lowest numbered vertex in patch
! (I = J = 1).
! CREDPT - BOTH
! Create both cells and vertices.
! VERT
! Create vertices only.
! CELL
! Create cells only.
! ICSRF - If ICSRF is non-zero, then the interior vertices are
! projected to the surface defined by shells of type ICSRF
! after the orthogonalizing pass (if any).
! NITER - If NITER > 0, then a routine is called to attempt to
! orthogonalize the newly created mesh. This routine also tends
! to flatten out the surface (if curved) and is best used on
! planar patches. It may, however, be used in conjunction with
! ICSRF' to smooth and place vertices onto a curved surface
! simultaneously.
```
APPENDIX D. INPUT-FILES

! TOL, RLXF - Tolerance and under-relaxation factor to apply to the orthogonalizer. These are ignored if NITER = 0.
! RATIQI,J - Each successive space between new vertices is RATIO x the previous space. Use ratio = 1.0 (default) for linear (even) spacing. If RATIO < 0, then use accordion fill (i.e. spacing increases to middle of fill and then decreases again to reach the second point).
! RATIQI determines spacing in the I (NV1 to NV2) direction, while RATIQJ determines spacing in the J (NV1 to NV4) direction.

! patch first 10 cm
patch 01 09 14 13 anz1 anz8
patch 09 10 15 14 anz2 anz8,,,,,,,,ra0878,ra10
patch 10 05 08 15 anz3 anz8,,,,,,,,1 / ra11,ra10
patch 06 11 16 07 anz5 anz8,,,,,,,,1 / ra08,ra10
patch 11 12 17 16 anz6 anz8
patch 12 02 18 17 anz7 anz8,,,,,,,,ra08,ra10
set anz3 2
set anz4 4
set anz5 2

! patch mixingzone
set mixrefine 2
patch 13 14 19 04 anz1 anz9,,,,,,,,ra10,ra10
patch 14 15 20 19 anz2 anz9,,,,,,,,ra0878,ra10
patch 15 08 21 20 anz3 anz9 + mixrefine,,,,,,,,1 / ra10,ra10
patch 08 07 22 21 anz4 anz9 + mixrefine,,,,,,,,ra10,ra10
patch 07 16 23 22 anz5 anz9 + mixrefine,,,,,,,,ra10,ra10
patch 16 17 24 23 anz6 anz9,,,,,,,,ra10,ra10
patch 17 18 03 24 anz7 anz9,,,,,,,,ra08,ra10

! patch L1-block
!*set anz3 1
!*set anz4 2
!*set anz5 1
*set anz1 L1 / znorm + 1
patch 04 19 26 25 anz1 anzL1
patch 19 20 27 26 anz2 anzL1,,,,,,,,ra0878,ra10
patch 20 21 28 27 anz3 anzL1
patch 21 22 29 28 anz4 anzL1
patch 22 23 30 29 anz5 anzL1
patch 23 24 31 30 anz6 anzL1
patch 24 03 32 31 anz7 anzL1,,,,,,,,ra08,ra10

! patch z1-block
patch 25 26 34 33 anz1 1
patch 26 27 35 34 anz2 1,,,,,,,,ra0878,ra10
patch 27 28 36 35 anz3 1
patch 28 29 37 36 anz4 1
patch 29 30 38 37 anz5 1
patch 30 31 39 38 anz6 1
patch 31 32 40 39 anz7 1,,,,,,,,ra08,ra10

! patch L2-block
D.3. 5° AND 25° MESH CREATION INPUT-FILE

*set anzL2 L2 / znorm + 1
patch 33 34 42 41 anzl anzL2
patch 34 35 43 42 anz2 anzL2,,.....,ra0878,ra10
patch 35 36 44 43 anz3 anzL2
patch 36 37 45 44 anz4 anzL2
patch 37 38 46 45 anz5 anzL2
patch 38 39 47 46 anz6 anzL2
patch 39 40 48 47 anz7 anzL2,,.....,ra08,ra10

! patch z2-block
patch 41 42 50 49 anz1 1
patch 42 43 51 50 anz2 1,.....,ra0878,ra10
patch 43 44 52 51 anz3 1
patch 44 45 53 52 anz4 1
patch 45 46 54 53 anz5 1
patch 46 47 55 54 anz6 1
patch 47 48 56 55 anz7 1,.....,ra08,ra10

! patch L3-block
*set anzL3 L3 / znorm + 1
patch 49 50 58 57 anz1 anzL3
patch 50 51 59 58 anz2 anzL3,,.....,ra0878,ra10
patch 51 52 60 59 anz3 anzL3
patch 52 53 61 60 anz4 anzL3
patch 53 54 62 61 anz5 anzL3
patch 54 55 63 62 anz6 anzL3
patch 55 56 64 63 anz7 anzL3,,.....,ra08,ra10

! patch z3-block
patch 57 58 66 65 anz1 1
patch 58 59 67 66 anz2 1,.....,ra0878,ra10
patch 59 60 68 67 anz3 1
patch 60 61 69 68 anz4 1
patch 61 62 70 69 anz5 1
patch 62 63 71 70 anz6 1
patch 63 64 72 71 anz7 1,.....,ra08,ra10

! patch L4-block
*set anzL4 L4 / znorm + 1
patch 65 66 74 73 anz1 anzL4
patch 66 67 75 74 anz2 anzL4,,.....,ra0878,ra10
patch 67 68 76 75 anz3 anzL4
patch 68 69 77 76 anz4 anzL4
patch 69 70 78 77 anz5 anzL4
patch 70 71 79 78 anz6 anzL4
patch 71 72 80 79 anz7 anzL4,,.....,ra08,ra10

vset all
vplo all
cset all

! Extrusion of Shell type cells to fluid cells over 5 degrees per slice
! For a 5 degree slice set slices to 1, for a 25 degree set slices to 5.
*set slices 5
ctyp 1
csys 2
vcex slices 5000 cset,,loca 0. 5. 0.

! Deletion of shells from which fluid were extruded
cset news shell
APPENDIX D. INPUT-FILES

cdel cset
numb vert off

! Merger of all cells, remaining cells are coupled (near mixing zone)

vmer,all,,0.0000001,,,,,low,delete,c
cset all
cptype, 2
chec,all,0,righ,news,noli $chec,all,0,righ,news,noli
chec,all,0,crack,0.0001,newset,nolist
cset all
cpmu,cset,,0.01,0.25,15,noset,novfix,2
view,-0.00555572,0.0111016,-l$angl,0.00176742$axis,y$dist,0.00386598
cent,0.00375002,0.000261552,6.17684e-06$pltb,on$cplot$pltb,off
vcomp $y $y
ccomp $y

D.4 90° × 120° mesh generation input-file

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! Cleansing of Tables !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
bdel all
cyde,1,1473,1
blkd all
del all
cdel all
cpdel all
vstyle,2,4,1
qdraw,edge
ccom $y

!!!!!!!!!!!!!!!!!!!!
! Creation of the Mesh !
!!!!!!!!!!!!!!!!!!!!
! Definition of Primary Vertices for Spline and Block Definition !

! Inner radius inlet tube
*set rl 5e-3

! Outer radius inlet tube
*set r2 5.59e-3

! Inner radius pipe
*set r3 7.5e-3

! Radial position 120° corner
*set s 4e-3

! End of inner tube
*set li 100e-3

! End of refined zone
*set 12 200e-3

! End of simulated pipe domain
*set 13 600e-3
! Radial position of 60° corners
*set p 0.8965 * s

! Switch to cartesian coordinates
csys 1
! Definition of center and 60° corners
v 1 0 0 0
v 2 p 0 0
v 3 0 p 0

! Switch to cylindrical coordinates
csys 2
! Definition of the 120° corner
v 4 s 45 0
! Definition of the inner wall of the inlet tube
v 5 r1 0 0
vgen 25 1 5 5 1 0 3.75 0
! Definition of the outer wall of the inlet tube
v 30 r2 0 0
vgen 25 1 30 30 1 0 3.75 0
! Definition of the inner wall of the pipe
v 55 r3 0 0
vgen 25 1 55 55 1 0 3.75 0

! Generation of vertices from z=0 to z=ll, z=12, z=1cross and z=13
vgen 2 100 1 79 1 0 0 11
vgen 2 200 1 79 1 0 0 12
vgen 2 300 1 79 1 0 0 13

! Definition of Splines
spl 1 vran 5 29
spl 2 vran 30 54
spl 3 vran 55 79

! Generation of Splines on basis of the defined splines
splg 2 3 1 3 1 100
splg 2 6 1 3 1 200
splg 2 12 1 3 1 300

! Block Definition and Execution: Creation of cells!
blk 1 1 2 4 3 101 102 104 103
blk 2 101 102 104 103 201 202 204 203
blk 3 201 202 204 203 301 302 304 303

! The parameter n12 controls the coarseness of the
! mesh. Set at 10 the input file generates a 10X10
! mesh, set at 8 or 5 it generates, respectively the
! 8X8 or a 5X5 mesh.
*set n12 8
*set n13 n12 / 1
*set z11 20
*set z12 25
*set z13 70
*set r12 1.
*set r13 1.
*set rz1 0.96
*set rz2 1.03
*set rz3 0.995
blkf,1,n13,n13,z11,0,0,0,r12,r13,rz1
blkf,2,n13,n13,z12,0,0,0,r12,r13,rz2
blkf,3,n13,n13,z13,0,0,0,r12,r13,rz3
blk 4 2 5 17 4 102 105 117 104
APPENDIX D. INPUT-FILES

D.5  $90^\circ \times 120^\circ$ Simulation setup

!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! Creation of the Mesh !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!

! Execute commands of the mesh generation input file
! such as in the previous section.

ifile 90o8.inp

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! Definition of Problem !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! One phase simulation in accordance with experimental
! data of 23-10-2002

*set Tinner 284.55
*set Touter 321.15
*set vinner 2.78
*set vouter 2.78
D.5. \(90^\circ \times 120^\circ\) SIMULATION SETUP

\[
\text{\(k_{in}=1.5(U*I)^{-2}\), where } U \text{ is the inlet velocity and } I \text{ is the turbulence intensity. } I \text{ is } 10% \\
\]

\*set \(k_{in} 0.159\)

\[
\text{\(\varepsilon_{inner}= C_{mu}^{-3/4} k_{in}^{-3/2} / l_{inner}\), where } C_{mu}=0.09 \\
\text{and } l_{inner} \text{ is the turbulent mixing length, approximately } 0.2*(\text{pipe radius}) \\
\]

\*set \(\varepsilon_{inner} 6.483\)

\[
\text{For the annular section } l_{outer} \text{ is set at 10\% of the distance between the inlet tube and the pipe wall.} \\
\text{\(l_{outer}=0.1*1.91E-3 \text{ m}\)} \\
\]

\*set \(\varepsilon_{outer}=33.94\)

\*set \(Sc 0.90\)

\*vstyle,2,4,1
\*qdraw,edge

！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！！
D.5. 90° × 120° SIMULATION SETUP

geom$
prob$
save$
Appendix E

User-codes

E.1 User-code DROICO.F for Steady State Analysis

The following code is one formulation of DROICO.F, because it is to be adapted for each simulation depending on mesh for the inlet area and on the simulated dispersed phase volume fraction. Randomization is carried out using RAND, so no high hopes should be had about the truly random nature of this scheme. Because theta and r are randomized separately, and area is quadratic in r, the root is taken of the RAND-value to ensure that the parcels are evenly distributed over the total area.

```
SUBROUTINE DROICO(IDRT,RNDP,XD,YD,ZD,UD,VD,WD,DRD,DENDR,TD,
& ICSRGP,OMEGRP)
C Droplet initial conditions
C******************************************************************************
C STAR RELEASE 3.150
C******************************************************************************
C This subroutine enables the user to specify droplet initial conditions.
C ** Parameters to be returned to STAR: IDRT, RNDP, XD, YD, ZD, UD, VD, WD, DRD, DENDR, TD ICSRGP, OMEGRP
C Droplet type IDRT is passed to this subroutine as a negative number.
C If its value is not changed to positive value (between 1 and 10) this subroutine will not be called and injection of particles will be held until the next time step.
C NP is the number of injected parcels, c.q. the number of tracks NP=20000
C Seeding the randomization on the first iteration IF(IDN.GT.NP) RETURN
```
APPENDIX E. USER-CODES

IF(IDN.EQ.1) THEN
WRITE(*,*) 'DROICO.F CALLED'
ENDIF

IF(ITER.EQ.1) THEN
call srand(981345672)
ENDIF

C Injected volume percentage dispersed phase, c.q. particles
VOLPERC=1E-4
ICSRGP=2
ONEGRP=0
IDRT=1

C INITIAL VELOCITY OF A DROPLET (m/s)
UD=0.0
VD=0.0
WD=2.78

C DROPLET DENSITY (kg/m3)
DENDR=2350
PI=3.1415927

C SWITCH TO OTHER DIAMETER AFTER A FRACTION OF PARCELS
FRACTION=0.79
IF(IDN.LE.(FRACTION*NP)) THEN
C DROPLET DIAMETER
DRD=60.E-06
C NUMBER OF PARTICLES PER SECOND
A=MASSFLOW_(FLUID,IN)/RHO_FLUID/(PI*DRD^3)
A=47677698
FLOWPART=VOLPERC/(100-VOLPERC)*A*FRACTION
C Calculation of the number of particles represented by a parcel.
RNDP=FLOWPART/NP/FRACTION
C WRITE(*,*) DRD,FLOWPART,RNDP
ELSE
C DROPLET DIAMETER
DRD=55.E-06
C NUMBER OF PARTICLES PER SECOND
A=MASSFLOW_(FLUID,IN)/RHO_FLUID/(PI*DRD^3)
A=208469673
FLOWPART=VOLPERC/(100-VOLPERC)*A*(1-FRACTION)
C Calculation of the number of particles represented by a parcel.
RNDP=FLOWPART/NP/(1-FRACTION)
C WRITE(*,*) DRD,FLOWPART,RNDP
ENDIF

C INITIAL POSITION OF DROPLET (m)
1 R=(7.5e-3-DRD)+SQRT(RAND())
IF((R.GE.(5e-3-DRD/2)).AND.(R.LE.(5.59e-3+DRD/2))) GOTO 1
THETA=(90*RAND())*pi/180
XD=R*cos(THETA)
YD=R*sin(THETA)
ZD=DRD/2

C DROPLET TEMPERATURE (K)
C FOR INNER INLET TUBE
IF((R.LE.(5e-3)).AND.(R.GE.(DRD/20))) THEN
TD=289.95
C FOR OUTER ANNULAR FLOW
ELSE IF((R.GE.(5.59e-3)).AND.(R.LE.(7.5e-3))) THEN
TD=328.95
ELSE
WRITE(*,*) R*1000,THETA*360/2/PI,IDN,'ERROR'
GOTO 1
ENDIF

RETURN
END
E.2. USER-CODE DROMOM.F

E.2 User-code DROMOM.F

SUBROUTINE DROMOM(DCO, VMC, BF)
C
C  Droplet momentum information
C
C******************************************************************************
C
C  INCLUDE 'comdb.inc'
C  INCLUDE '../parm.inc'
C
C23456789012345678901234567890123456789012345678901234567890123456789012
C
COMMON / DC02 / T(-NBMAX:NCTMAX,1+NSC)
C
C  T(IC,1):  Relative temperature in STAR cell/boundary IC
C  T(IC,1+IS):  Concentration of scalar IS in STAR cell/boundary IC
C
COMMON/USROOl/INTFLG(100)
C
DIMENSION BF(3)
C
INCLUDE 'usrdat.inc'
C
EQUIVALENCE( UDAT04(002), DEN )
EQUIVALENCE( UDAT04(059), U )
EQUIVALENCE( UDAT04(060), V )
EQUIVALENCE( UDAT04(061), W )
EQUIVALENCE( UDAT04(062), VISM )
EQUIVALENCE( UDAT06(003), DRD )
EQUIVALENCE( UDAT06(008), UD )
EQUIVALENCE( UDAT06(006), UD )
EQUIVALENCE( UDAT06(007), UD )
C
WRITE(*,*) 'IPSTAR=',IPSTAR
DUDXS=T(IPSTAR,2)
DVDXS=T(IPSTAR,3)
DWDXS=T(IPSTAR,4)
DUDYS=T(IPSTAR,5)
DVDYS=T(IPSTAR,6)
DWDYS=T(IPSTAR,7)
DUDZS=T(IPSTAR,8)
DVDZS=T(IPSTAR,9)
DWDZS=T(IPSTAR,10)

C This subroutine enables the user to calculate the drag coefficient, virtual mass coefficient and additional body force of droplets.

C ** Parameters to be returned to STAR: DCO, VMC and BF
C
C
C - DROPLET REYNOLDS NUMBER BASED ON RELATIVE VELOCITY
VR=SQRT((UD-U)**2+(VD-V)**2+(WD-W)**2)
RE=DEN*VR*DRD/VISM
C - DRAG COEFFICIENT - (DCO)
IF(RE.LE.1000.) THEN
   DCO = 24.*(1.+0.15*RE**0.687)/RE
ELSE
   DCO = 0.44
ENDIF
C - VIRTUAL MASS COEFFICIENT
VMC = 0
APPENDIX E. USER-CODES

C - The transverse lift force appears in literature in different forms.
C - In this file the formulation of Lain and Sommerfeld are implemented. Switching between formulation can be done by commenting and decommenting the appropriate lines.
C - Lain's formulation can be seen as a special case of the more general formulation of Sommerfeld. Therefore Sommerfeld is chosen for calculation.

C - Calculation of the Transverse lift force on basis of Lain's formulation
C
C \( C_1 = 0.5 \times \frac{3.1415927}{6} \times DRD \times DRD \times DRD \times DEN \)
C \( F_{TL1} = C_1 \times ((V - VD) \times (DUDYS - DVDXS) - (W - WD) \times (DWDXS - DUDZS)) \)
C \( F_{TL2} = C_1 \times ((V - VD) \times (DVDYS - DWDYS) - (U - UD) \times (DUDYS - DVDXS)) \)
C \( F_{TL3} = C_1 \times ((U - UD) \times (DVDZS - DWDYS) - (V - VD) \times (DVDZS - DWDYS)) \)
C - End of Lain's formulation

C - Calculation of the transverse lift force on basis of Sommerfeld's formulation
C Sommerfeld's formulation

C - Calculation of the particle Reynolds shear number
C 4 = DEN/VISH*DRD*DRD*SQRT((DVDXS+DWDXS)*(DVDXS+DWDXS)+
C & (DVDYS+DWDYS)*(DVDYS+DWDYS)+(DUDYS+DUDZS)*(DUDYS+DUDZS))
C  BETA=0.5*RES/RE
C IF(RE.LE.40.) THEN
C  F=(1-0.3314*SQRT(BETA))*EXP(-RE/10)+0.3314*SQRT(BETA)
C  CLS=4.1126*F/SQRT(RES)
C ELSE
C  IF(RE.GT.40.) THEN
C  CLS=4.1126*0.0524*SQRT(0.5)
C ELSE
C  WRITE(**,*) 'ILLOGICAL RE_P VALUE, NO CLS VALUE ASSIGNED'
C  WRITE(**,*) 'RE_p',RE
C  WRITE(**,*) 'MOLECULAR VISCOSITY',VISH
C  WRITE(**,*) 'PARTICLE DIAMETER',DRD
C  WRITE(**,*) 'FLUID DENSITY',DEN
C  WRITE(**,*) 'SLIP VELOCITY',VR
C ENDIF
C ENDIF

C - Lain's coefficient for \( C_{LS} \) is 2/3
C 4 = 0.5*3.1415927/6*DRD*DRD*DRD*DEN
C 4 = 4*CLS
C  FT1 = 4*((V - VD) \times (DUDYS - DVDXS) - (W - WD) \times (DWDXS - DUDZS))
C  FT2 = 4*((V - VD) \times (DVDYS - DWDYS) - (U - UD) \times (DUDYS - DVDXS))
C  FT3 = 4*((U - UD) \times (DVDZS - DWDYS) - (V - VD) \times (DVDZS - DWDYS))
C - End of Sommerfeld's formulation

C - SCREEN PRINT OF FIRST ITERATION VARIABLES
C
C IF (idr.EQ.1) THEN
C  WRITE( *, *) 'DROMM CALLED'
C  WRITE( *, *) 'IPSTAR=',IPSTAR
C  WRITE( *, *) 'C_LS=',CLS
C  WRITE( *, *) 'RE_p',RE
C  WRITE( *, *) 'RE_s',RES
C C WRITE( *, *) 'dudx',DUDXS
C C WRITE( *, *) 'duyo',DUDYS
C C WRITE( *, *) 'dwdx',DWDXS
C WRITE( *, *) 'dudy',DUDYS
C C WRITE( *, *) 'dwdy',DWDYS
C C WRITE( *, *) 'dudz',DUDZS
C C WRITE( *, *) 'dvdz',DVDZS
C C WRITE( *, *) '******************************************+
C C C END
C
C - ADDITIONAL FORCES PER UNIT TIME ACTING ON A DROPLET
E.3. USER-CODE SCALFN.F

SUBROUTINE SCALFN(PHI)

C Species-scalar function
C************************************************************
C ** Parameter to be returned to STAR: PHI
C
C This subroutine enables the user to specify SCALAR(IS) in
C an arbitrary manner, instead of solving the corresponding
C transport equation.
C
IF(IS.EQ.01) THEN
  PHI=DUDX
  WRITE(*,*), 'DUDX=', PHI
ELSE IF(IS.EQ.02) THEN
  PHI=DVDX
  WRITE(*,*), 'DVDX=', PHI
ELSE IF(IS.EQ.03) THEN
  PHI=DWDX
  WRITE(*,*), 'DWDX=', PHI
ELSE IF(IS.EQ.04) THEN
  PHI=DUDY
  WRITE(*,*), 'DUDY=', PHI
ELSE IF(IS.EQ.05) THEN
  PHI=DVDY
  WRITE(*,*), 'DVDY=', PHI
ELSE
  RETURN
ENDIF

RETURN
END
If(IS.EQ.06) THEN
  PHI=DWDY
  WRITE(*,*) 'DWDY=', PHI
ELSE
  IF(IS.EQ.07) THEN
    PHI=DUDX
    WRITE(*,*) 'DUDX=', PHI
  ELSE
    IF(IS.EQ.08) THEN
      PHI=DVDZ
      WRITE(*,*) 'DVDZ=', PHI
    ELSE
      IF(IS.EQ.09) THEN
        PHI=DWDZ
        WRITE(*,*) 'DWDZ=', PHI
      ELSE
        WRITE(*,*) '*************************************'
        WRITE(*,*) 'SCALFN CALLED WITHOUT ASSIGNING VALUE'
        WRITE(*,*) '*************************************'
      ENDIF
    ENDIF
  ENDIF
ENDIF
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E.4 User-code VISMOL.F

*************************************************************************
SUBROUTINE VISMOL(VISM)
C Viscosity (molecular)
*************************************************************************
C------------------------------------------------------------------------
C STAR RELEASE 3.150 
C------------------------------------------------------------------------
C INCLUDE 'comdb.inc'
COMMON/USRO01/INTFLAG(100)
C INCLUDE 'usrdat.inc'
DIMENSION SCALAR(50)
COMMON/SCALA/SCL(60)
EQUIVALENCE( UDAT11(007), T )
C------------------------------------------------------------------------
C This subroutine enables the user to specify the molecular viscosity
C (VISM) in an arbitrary manner.
C STAR calls this subroutine for boundaries and cells.
C ** Parameter to be returned to STAR: VISM
C The molecular viscosity's dependance on temperature is accounted
C for by a parabolic fit through empirical data.
C------------------------------------------------------------------------
VISM=(26.775E-3)-(1.5372E-4)*T+(2.2442E-7)*T*T
RETURN
END
Appendix F

Program files

F.1 Program TRACK_READER.F

```
PROGRAM TRACK_READER
C------------------------------------------------------------------------
C Reads the .trk files generated by Star-CD and
C writes them to an output file.
C------------------------------------------------------------------------
IMPLICIT NONE
LOGICAL DFLAG
CHARACTER FID*4, IDENT*4, FILENAME*80, OFILE*80
INTEGER I,IDRP,ICELL,JVERS
REAL X,Y,Z,U,V,W,DTIME,TDR,DDR,DMASS,CDR,DUM(11)
WRITE(*,30)
READ(*,'CA)') FILENAME
WRITE(*,31) FILENAME
READ(*,'CA)') OFILE
WRITE(*,28) OFILE
OPEN (UNIT=33, FILE=FILENAME, STATUS='OLD', FORM='UNFORMATTED')
OPEN (UNIT=85, FILE=OFILE, STATUS='UNKNOWN')
READ (33, ERR=910, END=900) FID, JVERS, IDENT, DUM(I), I=1,11
C Start of loop through track file
20 READ (33, ERR=910, END=900) IDRP, X, Y, Z, U, V, W, DFLAG, DTIME,
  & IDCELL, TDR, DDR, DMASS, CDR
  WRITE (85, 50) IDRP, X, Y, Z
  WRITE (85, 51) DFLAG, U, V, W
  WRITE (85, 52) IDCELL, DTIME, TDR, DDR
  WRITE (85, 53) DMASS, CDR
  WRITE (*, *) 'G' GO TO 20
900 CONTINUE
WRITE (*, *) 'END of my file'
CLOSE (85)
CLOSE (33)
STOP
C------------------------------------------------------------------------
30 FORMAT ('TYPE DROPLET FILE NAME:')
31 FORMAT ('DROPLET FILE NAME SELECTED: ', A)
27 FORMAT ('OUTPUT FILE NAME:')
28 FORMAT ('OUTPUT FILE NAME SELECTED: ', A)
50 FORMAT (14,3F10.5)
51 FORMAT (14,3F10.5)
52 FORMAT (14,3F10.5)
53 FORMAT (8F10.5)
C------------------------------------------------------------------------
910 WRITE (*, *) 'Error in my file'
```

147
STOP
END